

Two-Phase Detailed Numerical Modelling of Falling Film Evaporation Phenomena

by

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Abstract

Desalination has been recognized as a climate-independent source of producing potable water that has a great importance due to the lack of drinking water in many countries. One of the methods extensively used for removing salt from seawater is thermal distillation, which is known as a reliable technology for producing high-quality water through evaporation. Among different evaporation methods, a liquid falling film has been widely developed in the thermal desalination industry.

The flow characteristics of the falling evaporation process are complicated, and heat and mass transfer are strongly interdependent. Some previous numerical studies simplified the solution by using a boundary layer approximation, which is not capable of modelling reverse flows and recirculation zones. The previous models that solved the full governing equations (elliptic approach) applied the volume of fluid method (VOF), which is not able to precisely determine the location of the liquid and gas interface, therefore, it cannot accurately apply the interface jump conditions. Additionally, these studies commonly used mass transfer models based on estimations and empirical correlations, which introduce limitations to numerical simulations. Another limitation found in the previous studies is that none of them has considered the occurrence of the supersaturation phenomenon in the mixture phase, which may occur during the evaporation process.

In this research, a two-dimensional, two-phase model was developed using an in-house Fortran code that solves the steady-state, full elliptic governing equations for the liquid and gas phases. This modeling represents a significant advancement in the simulation of the evaporation phenomenon that employs innovative methods to address the aforementioned problems. This model is believed to be the most comprehensive and detailed approach compared to any previous numerical studies on falling film evaporation. A variety of boundary conditions and geometries have been utilized to analyze the details of evaporation and desalination phenomena. The results were then compared to available experimental and numerical data for validation purposes. In each stage, a new set of detailed results, including the effects of different parameters variation on flow characteristics and heat and mass transfer during the evaporation process are presented.

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Dedication

To my beloved family,
for their endless love, support, and encouragement through every step of this journey.

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Nomenclature

A	area, [m ²]
A, a, B, b	coefficients in the algebraic equations
A_x, A_y, B_x, B_y	geometric parameters
$\tilde{b}$	source term in PWIM equations
C	coefficient for interpolations of corner values
C_p	specific heat, [J kg ⁻¹ K ⁻¹]
D	tube diameter, [m]
D^{AB}	binary diffusion coefficient, [m ² s ⁻¹]
$\tilde{d}$	weight function in PWIM equations
ds	distance along $\hat{s}$ vector for a single control volume, [m]
dt	distance along $\hat{t}$ vector for a single control volume, [m]
E	E-factor
E^*	dimensionless parameter in Equation (B.3)
f	interpolation coefficient
Fr_L	liquid Froude number ($\overline{U}_{L,in}^2/(g \delta_{in})$)
Gr_M	local mass Grashof number, Equations (6.2) and (8.5)
Gr_Q	wall heat flux Grashof number, Equation (5.10)
Gr_T	local thermal Grashof number, Equations (6.1) and (8.4)
g	gravitational acceleration, [m s ⁻²]
H	channel or domain half width, [m]
h_{fg}	latent heat of vaporization, [J kg ⁻¹]
h	overall heat transfer coefficient, [W m ⁻² K ⁻¹]
$\bar{h}$	partial mass enthalpy, [J kg ⁻¹]
h_L	interface height, [m]
h_v	water vapour enthalpy, [J kg ⁻¹]
i	index in the x or χ direction
$\hat{i}$	normal unit vector in the x direction

Nomenclature

i_B, i_E	first, last control volume indices in the x or χ direction
J	mass flow rate through a control volume north face, $[\text{kg s}^{-1}]$
J''	mass flux through a control volume north face, $[\text{kg m}^{-2} \text{s}^{-1}]$
J^*	dimensionless parameter in Equation (B.2)
j	index in the y or η direction
$\hat{j}$	normal unit vector in the y direction
j_B, j_E	first, last control volume indices in the y or η direction
j_{BL}, j_{EL}	first, last control volume indices in the liquid in the y direction
j_{BG}, j_{EG}	first, last control volume indices in the gas in the y direction
jL, jG	index in the y or η direction in the liquid, gas
K	curvature of the interface, $[\text{m}^{-1}]$
k	thermal conductivity, $[\text{W m}^{-1} \text{K}^{-1}]$
k_B	Boltzmann constant
L	channel length, $[\text{m}]$
L_1	inlet to tube wall length, $[\text{m}]$
L_2	tube wall to outlet length, $[\text{m}]$
L_h	heated wall length, $[\text{m}]$
L_i	insulated wall length, $[\text{m}]$
M	molecular weight, $[\text{kg kmol}^{-1}]$
$\dot{m}$	mass flow rate, $[\text{kg s}^{-1}]$
$\dot{m}'$	mass flow rate per unit depth, $[\text{kg m}^{-1} \text{s}^{-1}]$
$\dot{m}''$	mass flux, $[\text{kg m}^{-2} \text{s}^{-1}]$
N_A	Avogadro's number
Nu_{intf}	Nusselt number at the liquid-gas interface, Equation (5.1)
N_x	number of nodes in the x direction
N_y	number of nodes in the y direction
n	normal direction

Nomenclature

$\hat{n}$	normal unit vector: $n_x\hat{i} + n_y\hat{j}$
P	pressure, [N m ⁻²]
q''	heat flux, [W m ⁻²]
q''_{ref}	reference heat flux, [W m ⁻²] ($k_L(T_{L,\text{in}} - T_{\text{wall}})/\delta_{\text{in}}$)
$\mathcal{R}$	algebraic equation residual
Re_M	mixture Reynolds number for channel ($\rho_G \overline{U}_{G,\text{in}} 2(H - \delta_{\text{in}})/\mu_G$)
$\text{Re}_{M,d}$	mixture Reynolds number for tube ($\rho_G \overline{U}_{G,\text{in}} d/\mu_G$)
Re_L	film Reynolds number ($4\rho_L \overline{U}_{L,\text{in}} \delta_{\text{in}}/\mu_L$)
S	grid geometric expansion factor
SR	supersaturation ratio
s	west to east node-to-node and node-to-face direction
$\hat{s}$	west to east geometric grid unit vector: $s_x\hat{i} + s_y\hat{j}$
Sh_{intf}	Sherwood number at the liquid-gas interface, Equation (5.2)
T	temperature, [K]
t	time, [s]
t	south to north node-to-node and node-to-face direction
$\hat{t}$	south to north geometric grid unit vector: $t_x\hat{i} + t_y\hat{j}$
U	velocity in the x direction, [m s ⁻¹]
V	velocity in the y direction, [m s ⁻¹]
$\vec{V}$	velocity vector, [m s ⁻¹], $U\hat{i} + V\hat{j}$
$\vec{V}_t$	tangential velocity, [m s ⁻¹]
∇	volume of a control volume, [m ³]
W	mass fraction
$\mathcal{W}$	geometric linear interpolation factor
x, y	Cartesian coordinate directions, [m]
$\mathcal{X}, \mathcal{Y}$	geometric parameter for calculation of gradient

Greek Letters

α	convective weighting coefficient
β	diffusive weighting coefficient
Γ	gradient value at the boundary
γ	geometric parameter
δ	film thickness, [m]
ε	effectiveness, Equations (5.11) and (6.5)
ϵ	steady state convergence criterion
η	transformed transverse coordinate
θ	tube central angle [rad]
μ	dynamic viscosity, [kg m ⁻¹ s ⁻¹]
ρ	density, [kg m ⁻³]
σ	surface tension, [N m ⁻¹]
τ	stress tensor, [N m ⁻²]
Φ	general variable (referring to U , V , J , P , T , or W)
ϕ	relative humidity (also referred to as RH)
χ	transformed axial coordinate
Ψ	maximum percent difference

Subscripts

a	referring to air in the gas phase
b	referring to bulk value
bnd	referring to domain boundary
e, w, n, s	referring to quantities at the east, west, north, south face of a control volume

Nomenclature

E, W, N, S	referring to quantities at the east, west, north, south nodal points
G	referring to the gas
i	west to east control volume index
iG	referring to quantities at the gas interface
iL	referring to quantities at the liquid interface
in	at the inlet
intf	at the interface
j	south to north control volume index
L	referring to the liquid
M	referring to the mixture
NB4	referring to E, W, N, S
NB8	referring to NB4 and NE, NW, SE, SW
ne, nw, se, sw	referring to quantities at the northeast, northwest, southeast, southwest of a control volume
NE, NW, SE, SW	referring to quantities at the northeast, northwest, southeast, southwest nodal points
out	at the outlet
P	referring to the node
sat	saturation condition
spec	referring to a specified value
SSL	supersaturation limit
tot	total amount
v	referring to the vapour
W	referring to water in the solution
wall	at the wall
xe	referring to the x component of a vector on the east face
xn	referring to the x component of a vector on the north face

xP	referring to the x component of a vector on the node
ye	referring to the y component of a vector on the east face
yn	referring to the y component of a vector on the north face
yP	referring to the y component of a vector on the node

Superscripts

c, u, v, t, W	referring to continuity, U , V , energy, and mass fraction equations
n	referring to the current iteration or time step
o	referring to the previous iteration or time step
ϕ	referring to a general transport parameter
-	referring to an average value

Miscellaneous

BTDMA	block-tridiagonal matrix algorithm
CV	control volume
ILMB	Integral Liquid Mass Balance
ip	integration point
PETSc	The Portable, Extensible Toolkit for Scientific Computation
PWIM	Pressure-Weighted Interpolation Method

Chapter 1

Introduction

1.1 Overview

Falling film evaporation is a dominant process in many practical applications such as desalination, refrigeration, electronics cooling, and food processing. Film evaporation is used in different applications with different working principles, and the main objective in all applications is the evaporation of some working fluid. For example, in cooling applications, the evaporation process is a mechanism for heat removal from a hot surface. In contrast, it is a means of mass transfer in the desalination industry to convert seawater into drinking water and water suitable for agricultural purposes. Also the evaporation process is used in pharmaceutical, petrochemicals, food industries such as sugar and baby formula production to achieve a desired mass concentration.

The evaporation process provides advantages such as high efficiency in small temperature differences, small pressure losses, and short residence time. The most common form of evaporation is film-wise, which occurs when a thin liquid film in the vicinity of a gas layer covers the entire surface of a wall or tube in a device called a falling film evaporator.

There are two common geometries used in industrial falling film applications: inside vertical tubes or channels and over horizontal tubes. Figure 1.1 shows the domain for the simulation of two-phase flow inside a channel. The falling liquid film flows along the wall surface, exposed to a uniform heat flux or temperature. In this case, the gas stream is forced to flow downwards. The applied heat flux leads to the partial evaporation of the liquid film and heat and mass transfer in the system. Vertical channel geometries are often used in microelectronic devices, combustion chambers, and cooling towers to transfer heat by latent energy transport during the evaporation process of a liquid film (evaporative cooling). Also, the vertical tube geometries are used in producing juice concentration and solvent removal.

Falling film evaporators require a large heat transfer surface area to achieve efficient evaporation. The size of an industrial falling film evaporator can vary depending on the specific application, capacity requirements, and design considerations. Falling film evaporators are commonly sized based on their evaporation capacity, which can range from small-scale systems, processing a few hundred liters per hour, to large industrial units, handling several thousand liters per hour. For example, an industrial desalination unit, with a capacity of 800,000 liters per hour, can provide the urban water for 100,000 people daily. The size of the evaporator unit depends on the capacity and the number of evaporation stages. In a desalination plant, for example, there might be thousands of horizontal tubes in each unit. The length of each tube can be between 3 and 10 m, and the diameter varies between 10 and 20 cm.

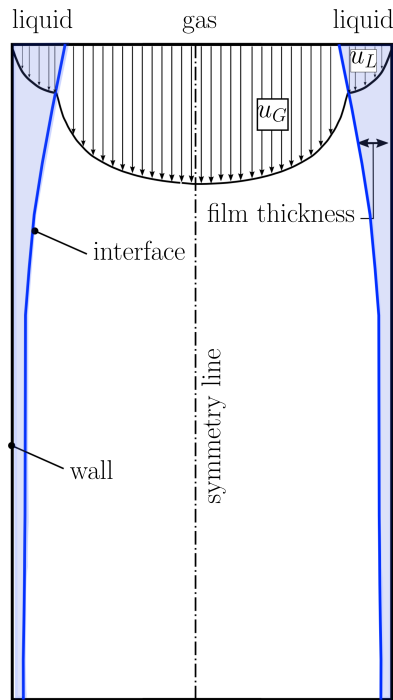


Figure 1.1: Domain for two-phase evaporation in a vertical channel

The domain of falling liquid film over a horizontal tube is shown in Figure 1.2. A thin liquid flows on the tube surface exposed to a uniform heat flux or temperature, and a gas stream flows downwards in the vicinity of the film. As the liquid film flows over the tube, its thickness decreases

due to the evaporation of the liquid. The principles of evaporation phenomenon are similar to those observed with the vertical channel; however, for a horizontal tube, the thickness of the liquid film varies and experiences thinning and thickening around the tube. This variation is influenced by the geometry curvature, the effect of gravity, and the effects of the gas stream. Tracking the film thickness in the grid generated around the tube is a significant challenge in numerical modeling of this phenomenon. The complexity arises from several factors such as the tube geometry, the shape of the liquid film, particularly at the upper and lower part of the tube, the tube surface wetting, and the droplet or jet formation between the tubes. All these factors contribute to the complexity of evaporation phenomenon over tubes. The horizontal tube geometries are utilized in the desalination and food industries.

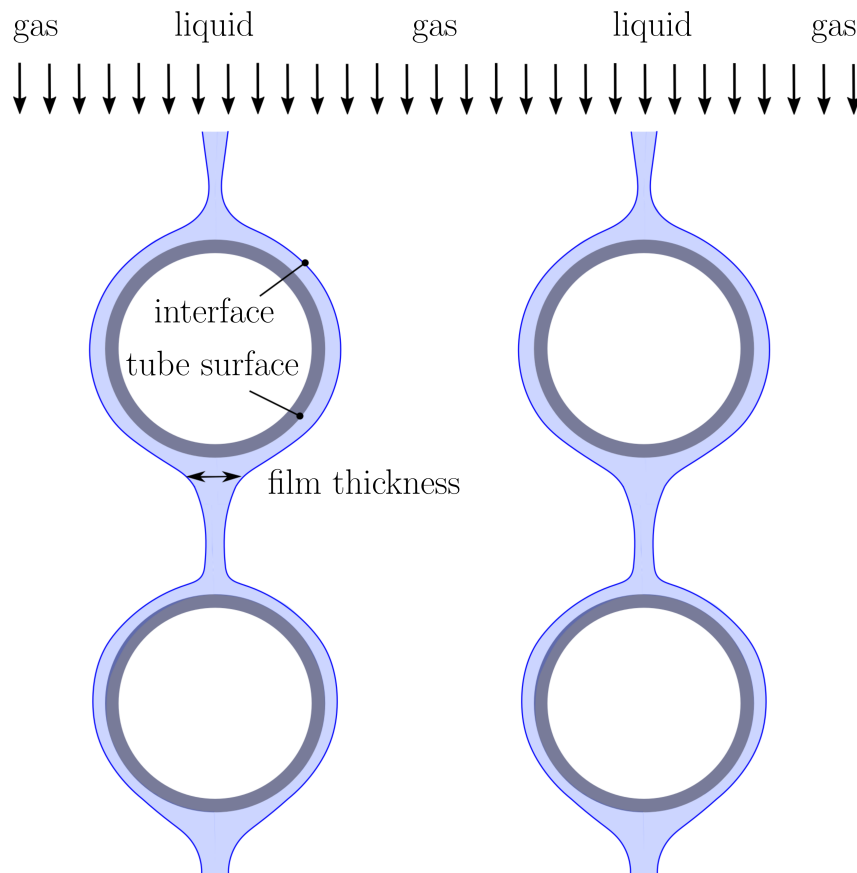


Figure 1.2: Domain for two-phase evaporation over horizontal tubes

1.1.1 Evaporation Phenomena

In two-phase flow systems, the heat and mass transfer in the liquid film are affected by the interface shear force and the energy and mass transfer rates. For the gas phase, besides the interfacial shearing force and vaporization rate, the effects of buoyancy forces can affect the flow behaviour. A key difference between falling film evaporation and condensation is the effects of buoyancy forces. In a condenser with a heavier non-condensing gas in a vertical geometry, the result of buoyancy effects is always downward. In an evaporator, however, the gas phase flow can move upwards or downwards depending on the thermal buoyancy and solutal buoyancy forces. For instance, for a system whose liquid film is water in the presence of air, the solutal buoyancy acts upwards because the molecular weight of water vapour is smaller than that of the air. Also, the thermal buoyancy always acts upwards due to the higher wall temperature compared to the ambient temperature. In the case of quiescent gas flow at the inlet, it can be difficult to determine the induced flow direction. In this regard, heat and mass transfer Grashof numbers are used as indicators of the relative strength of the buoyancy forces. If the sum of heat and mass transfer Grashof numbers is negative, the gas stream and liquid film flow downwards. Otherwise, the flow reversal will occur in the gas stream. To capture flow reversal, fully elliptic governing equations must be solved over the entire domain simultaneously.

1.1.2 The Desalination Process

Access to high-quality drinking water remains a significant challenge in many countries around the globe. Despite over two-thirds of the Earth's surface being covered by oceans, the high salinity levels makes this water undrinkable. To address this issue, the desalination industry has been significantly developed in recent years, aiming to provide solutions for accessing potable water. The most common methods used in the desalination industry are categorized into two main groups: those based on water filtration and those based on distillation. The former is more effective in areas with mild weather where energy costs are considerable, such as North America and Europe,

while the latter is used in hot areas where the water salinity is high and energy is more affordable, like Middle East. The most common form of filtration method is Reverse Osmosis (RO). This method operates based on a pressure difference on two sides of a semi-impermeable membrane, which prevents salt from passing through it. Some common issues in RO plants include membrane scaling and the presence of suspended solid particles in the produced desalinated water. In the absence of a practical non-thermal desalination system for high salinity levels, thermal methods are introduced to enhance process efficiency. There are three different technologies used in thermal desalination plants that rely on the distillation process and phase change for separation: multi-stage flash (MSF), mechanical vapour compression (MVC), and multi-effect distillation (MED). In MSF systems, salt water is preheated by an external energy source and then vaporized in a flash chamber due to expansion. The produced steam condenses on the outside surface of horizontal tube bundles, and the distilled water is collected in a tray. The remaining saltwater, called brine, is then passed to the next flash chamber with lower pressure. In MVC systems, seawater falling film usually flows over iso-thermal vertical parallel plates and is evaporated to the gas phase. The brine stream is also partially mixed with the seawater film and flows over the plate again. The MED system is an evaporator containing horizontal tube bundles where seawater flows over the external tube surface and is evaporated through different stages. The working temperature in MED is up to 70°C to reduce the risk of scaling, which acts as a thermal-resistant layer affecting the system efficiency.

1.2 Problem Statement

The objective of this research is to develop detailed numerical models, solving both parabolic and elliptic governing equations, to study the evaporation of a pure water or salt water falling film, in the presence of a gas stream, flowing inside a vertical channel or over a horizontal tube.

1.3 Literature Review

The topic of evaporation has been of interest to many researchers who used analytical, numerical, and experimental methods to study this complex phenomenon. During evaporation, the heat and mass transfer occur simultaneously. The gas phase flow may be laminar or turbulent, but the falling film flow is almost always laminar. The liquid and gas flow can be co-current or counter-current, depending on the combined forced and natural convection effects. Previous studies have been carried out on the effects of the vaporization mechanism, soluble material, binary mixture falling film, enhanced surface shape, and fouling on the evaporation process. In this review, the previous studies of falling film evaporation and desalination are classified into two main groups: numerical and experimental. The review is carried out in detail for the cases of flow evaporation in vertical parallel plate channels and over horizontal tubes.

1.3.1 Numerical Studies

There are two numerical approaches for the simulation of the evaporation process. In the first approach, the liquid film is assumed to be extremely thin and regarded as a boundary condition for heat and mass transfer for the gas phase. Therefore, the liquid transport equations are neglected. In the second approach, the liquid film has a finite thickness, so the transport equations are solved for both the liquid and gas phases. In a two-phase model, equations are solved for mass momentum, and energy transport in each phase. Sometimes, the equations are simplified, and the interface may be approximated or accurately resolved. The first part of this section is a review of numerical methods presented in the literature for falling film evaporation on vertical plates and inside vertical plate channels and vertical tubes. In the second part, the numerical studies of flow evaporation over horizontal tubes are summarized.

1.3.1.1 Numerical Studies: Vertical Channel Geometry

Preliminary numerical studies in this area considered an extremely thin film thickness, neglecting the effects of momentum and energy transport equations in the liquid phase [6–8]. The validity of an extremely thin film thickness assumption was examined by Yan [9]. For ethanol or water films in air, Yan solved a set of parabolic transport equations for both phases and neglected the inertial terms in the momentum equation for the liquid phase. He concluded that the assumption of the extremely thin thickness is valid only for low liquid mass flow rates. His study was extended to investigate the effects of the vaporization mechanism on the heat and mass transfer characteristics of test cases with different working conditions [10–14].

Tsay et al. [15] utilized a numerical approach to study the detailed heat transfer characteristics for a falling liquid ethanol film in air. The convection terms in the liquid momentum equation were considered negligible compared with the body force. Streamwise gradients of velocity and temperature were also considered much smaller than those in the transverse direction. Because the molecular weight is greater for ethanol than for air, the solutal buoyancy acts downwards due to ethanol evaporation, and reverse flow does not occur in this case. They found that a higher liquid inlet temperature and a lower liquid flow rate led to a more significant temperature drop of the liquid film. They also found that, for an insulated system with equal liquid and gas temperature, sensible heat transfer in the film and gas flow could occur due to the film vaporization because of the higher mass fraction of ethanol vapour at the interface than in the ambient. This mass fraction difference causes a mass diffusion of ethanol and consumes a considerable amount of energy by latent heat transport. The liquid film and gas flow supply this energy through sensible heat loss, and both phases are gradually cooled.

Tsay and Lin [16] conducted research on the numerical modelling of falling film evaporation of water on a vertical plate using simplified equations for the liquid phase, as in [15]. They applied a marching scheme in their simulations and showed that the approach only works for a limited range of heat flux and a small temperature difference between the liquid and gas flow. When the

gas velocity was not high enough, the combined buoyancy effects caused a flow reversal for a high rate of evaporation. It should be noted that the complete simulation of this situation requires the solution of the elliptic governing equations. Tsay and Lin also found that the evaporative latent heat transfer was the dominant heat transfer process between two phases and it depended mainly on the inlet liquid temperature and wall heat flux.

He et al. [17] conducted research to investigate the effects of mixed convection turbulent flow inside a vertical tube heated with a uniform heat flux. The falling film of water was assumed to be laminar. They concluded that, depending on the inlet water temperature, the energy supplied by the wall is used for either evaporation or direct film cooling. They showed that the wall and mixture temperature increased along the tube length when the water temperature was relatively high. Because the wall temperature was higher than the mixture temperature, the heat diffused away from the wall, and evaporation occurred. If the water temperature was relatively low and the mixture temperature was higher than the wall temperature, the heat diffused from the mixture towards the interface, and the advection of heat by the liquid falling film was the primary mechanism for heat removal from the tube surface.

Feddaoui et al. [18–21] and Feddaoui and Mir [22] numerically studied the effects of mixed convection on the heat and mass transfer of laminar and turbulent flows with different geometries and boundary conditions. They used a parabolic coupled-equation solution and concluded that the cooling of the liquid film is essentially affected by the latent heat transfer connected to the evaporation of the liquid film. A higher cooling rate was observed by increasing the inlet liquid temperature or decreasing the liquid mass flow rate.

Raach and Mitrovic [23] studied the evaporation of a seawater falling film on a vertical plate with turbulence-generating wires. They numerically investigated the effects of turbulence wires that were immersed in the falling film. They also utilized Nusselt's one-dimensional model for the evaporation of falling film without wires to study the impacts of salinity. Employing a VOF approach and a low Reynolds number k - ϵ model in the liquid film, they showed that the salt mass

fraction increases close to the interface due to evaporation of liquid water into the gas phase and to impermeability to salt. They also found that the heat transfer increases significantly by using turbulence-generating wires.

Raach and Mitrovic [24] also performed research on the numerical simulation of a conjugate heat transfer system using a 1-D and a 2-D program. They used falling seawater falling film as the working fluid over a vertical plate, heated by condensing water vapour. They examined the heat transfer between the condensing water film and the evaporating seawater flowing on each side of a conductive metallic plate. A comparison of the results obtained from 1-D and 2-D models demonstrated that both models were capable of capturing the main features of the falling film evaporation process. Therefore, the 1-D model was selected to use due to its computationally affordability and sufficiency for practical applications.

The evaporation of a binary (water-ethylene glycol) liquid film inside a vertical channel was investigated by Nasr et al. [25]. Using the boundary layer assumptions and a finite difference method, they showed that the heat and mass transfer depended greatly on the inlet concentration of ethylene glycol. Also, the water evaporation rate, in the case of the liquid mixture, could be higher than that for pure water.

Nait Alla et al. [26] studied the effects of partially heated walls on the heat and mass transfer in the evaporation of ethanol liquid film in a vertical channel. The partially heated plate was divided into sequential heated and insulated sections. An implicit finite difference method was applied to solve the coupled parabolic governing equations for liquid and gas phases. They found that the evaporation is more intensified when the insulated section is located at the channel exit. They also found the same conclusion as in [20] regarding the importance of latent heat exchange.

Ren and Wan [27] presented an elliptic numerical solution for modelling the laminar counter-current flow inside a vertical channel. Commercial CFD code Fluent was utilized for a 2-D model of the liquid and gas phases. They used a Nusselt solution to determine the initial water film thickness. A 1-D model was developed and applied to examine the average Nusselt and Sherwood

numbers based on the numerical results of the 2-D model.

Najim et al. [28] studied the heat and mass transfer of a salt water solution inside a vertical tube using a marching procedure. The simulation process was similar to that used by Feddaoui et al. [20]. Using a finite difference method, they determined the effect of pressure, liquid flow rate, tube length and wall heat flux on the performance of the desalination process.

Najim et al. [29] performed a study on a cooling approach using binary mixtures inside a vertical mini channel. They compared the evaporation of different mixture compositions to identify the appropriate mixture for the cooling purpose, and concluded that the higher concentration of water at the inlet leads to a higher efficiency with fewer thermal and mass losses.

Nait Alla et al. [30] carried out numerical modelling to investigate the process of evaporating liquid film mixture of water and ethanol inside a vertical channel and studied the effects of inlet water mass fraction, wall heat flux, and inlet liquid flow rate. They concluded that the heat and mass transfer for the binary water-ethanol liquid mixture can be enhanced for the high amounts of liquid ethanol at the inlet.

Nait Alla et al. [31] investigated the effects of a ternary liquid mixture along the channel wall. They showed that the high mass fraction of the volatile component and preheating of the liquid film improve the efficiency of the system.

Tohidi and Ormiston [32] conducted a numerical analysis of evaporation from a laminar falling liquid film with a co-current laminar gas-vapour mixture flow in a vertical parallel plate channel. A finite volume method was used to obtain a fully coupled implicit solution of a complete set of parabolic two-phase governing equations. Water and ethanol falling films were used in order to study the effects of the buoyancy forces in the system. They also investigated the effects of wall heat flux, relative humidity, and the inlet pressure on the heat and mass transfer of the system.

Tohidi and Ormiston [33] numerically investigated mixed convection effects on the flow and thermal characteristics of pure water falling film evaporation in a partially heated vertical channel. They employed elliptic governing equations and sharp interface tracking and developed a

methodology to account for supersaturation. They showed that strong thermal and solutal opposing buoyancy forces can induce reverse flow.

Nait Alla et al. [34] used a finite difference method and parabolic governing equations to study the impacts of nanoparticles on the desalination process for a falling liquid film inside a vertical channel. They concluded that adding the nanoparticles into the liquid film increased the evaporation rate due to the change in thermophysical properties.

A two-phase laminar flow model for the simulation of a thermal desalination process was presented by Tohidi and Ormiston [35]. They employed a finite volume approach and a sharp interface tracking method for a set of elliptic governing equations in both liquid and gas phases. They investigated the effects of inlet liquid Reynolds number, wall heat flux, salinity, and air relative humidity on the details of the flow and heat and mass transfer for falling film thermal desalination in a vertical parallel plate channel. Their results indicate that an increase in the inlet salinity leads to a reduction in the interfacial evaporation rate. Also, the effects of wall heat flux and inlet liquid Reynolds number changes on the flow, heat transfer, and mass transfer are more pronounced than the effects of changes in inlet salinity.

A summary of the numerical studies in vertical channels and tubes is presented in Table 1.1.

Table 1.1: Review of numerical studies of flow inside vertical channels

Author(s)	Year	Phases modeled	Solution method ^a	Wall B.C. ^b	Liquid film
Chang et al. [6]	1986	one	P	UWT	water
Lin et al. [7]	1988	one	P	A	water
Yan et al. [8]	1989	one	P	UWT	water
Tsay et al. [15]	1990	two	P	A	ethanol
Yan [9]	1992	one/two	P	UHF	water/ethanol
Tsay and Lin [16]	1995	two	P	UHF	water
He et al. [17]	1998	two	E	UHF	water
Feddaoui et al. [18]	2001	two	P	A	water
Feddaoui et al. [19]	2003	two	P	A	water
Raach and Mitrovic [23]	2005	one	VOF	UHF	seawater
Feddaoui et al. [21]	2006	two	P	A	water
Raach and Mitrovic [24]	2007	one	VOF	A	seawater
Feddaoui et al. [22]	2007	two	P	UHF	water
Nasr et al. [25]	2011	two	P	UHF	water
Nait Alla et al. [26]	2015	two	P	UHF/A	ethylene glycol
Ren and Wan [27]	2016	two	E	A	ethanol
Najim et al. [28]	2017	two	P	UHF	water
Nait Alla et al. [30]	2018	two	P	UHF/A	water/seawater
Nait Alla et al. [31]	2021	two	P	UHF/A	water/ethanol
Tohidi and Ormiston [32]	2022	two	P	UHF	water/methanol
Tohidi and Ormiston [33]	2023	two	E	UHF	benzene
Nait Alla et al. [34]	2023	two	P	UHF	water/ethanol
Tohidi and Ormiston [35]	2024	two	E	UHF	water
					seawater
					seawater

^a Method; P: Parabolic, E: Elliptic^b B.C. (Boundary Condition); UWT: Uniform Wall Temperature, A: Adiabatic, UHF: Uniform Heat Flux

1.3.1.2 Numerical Studies: Horizontal Tube Geometry

Falling film evaporation over a horizontal tube provides a higher heat transfer coefficient compared to a vertical channel system, therefore it has been more recommended for practical applications.

One of the prominent criteria in a horizontal tube setup, is the flow mode which has an important impact on the surface wetting and heat transfer characteristics of a liquid falling film over a horizontal tube. Generally, there are three different patterns of the liquid falling film flowing over a horizontal tube surface: droplet, column, and sheet, which are known as the main stable flow modes and characterized by the liquid mass flow rate, tube spacing, tube shape, and type of the working fluid. There are many experimental and numerical works studying the flow pattern transitions. For example, Mitrovic [36] reported that the transition from droplet to column and from column to sheet occurs at Reynolds numbers above 150 and 315, respectively.

A literature review has been conducted on previous numerical works studying the flow characteristics and evaporation of falling film over horizontal tubes. They used either CFD in-house codes or commercial software to perform the simulations. In all those studies that used a commercial code, the Volume of Fluid (VOF) method has been used to determine the location of the two phases.

Many researchers have conducted numerical studies under adiabatic conditions to analyze the flow hydrodynamics over horizontal tubes. Both 2-D and 3-D models have been employed in these simulations. Studies using a 3-D model primarily investigated the flow distribution in the third dimension [37, 38]. Conversely, scholars using a 2-D model typically focused on flow parameters and operational conditions in the simulations. Sun et al. [39] studied the effects of liquid film mass flow rate and feed height on the thickness and velocity distribution of a liquid falling film around a horizontal tube surface. They utilized a numerical method employing the VOF technique on a two-dimensional configuration using the commercial code ANSYS Fluent. They concluded that the liquid feed height is of great importance in the formation of the liquid falling film, and a shorter height leads to the formation of a smooth and continuous liquid film. Additionally, an increase in the liquid mass flow rate results in an increase in velocity and decrease in the film thickness around the tube.

Qiu et al. [40] utilized a two-dimensional VOF model to investigate the liquid falling film under

adiabatic conditions. They concluded that increasing the tube diameter reduces the film thickness; however, when the diameter of the tube becomes greater than a critical value, its impact on the liquid film, and thereby on the heat transfer, is not significant. They also showed that the minimum film thickness could occur at angles between 100 and 140 degrees from the top of the tube.

Qiu et al. [41] investigated changes in the liquid water film thickness on the surface of two in-line adiabatic horizontal tubes using VOF approach. They observed that the film thickness increases at the upper stagnation point with increasing liquid Reynolds number, but this can lead to the formation of a dry zone near the lower stagnation point due to the early departure of the liquid from the surface, which could cause fouling and negatively affect the heat transfer in a falling film evaporator. On the other hand, in the lower stagnation point region, for smaller liquid Reynolds numbers, the location where the liquid film departs from the surface shifts downwards, and the film remains longer on the surface of the tube.

The effects of spacing between two in-line tubes on the film thickness was investigated by Hassan et al. [42]. They utilized a two-dimensional VOF approach for the simulation of pure water falling film and observed that the film thickness is reduced by increasing the tube spacing.

Li et al. [43] conducted research on falling film flow over a horizontal tube with the liquid film exposed to counter-current gas flow. They utilized a 3-D configuration in ANSYS Fluent. Their simulations encompassed a wide range of liquid Reynolds numbers and gas flow rates. The results indicate that increasing the gas flow rate increases the bulk film thickness. They also analyzed various flow patterns, including droplet, jet, and sheet modes, and their effects on the distribution of film thickness over the tube surface.

Han et al. [44] used a 2-D transient numerical model using VOF approach to investigate the effects of tilting on the liquid film distribution around a horizontal tube. They observed that increasing the tilt angle reduces the film thickness at the top of the tube.

Lin et al. [45] utilized the VOF method to simulate falling film flow over a rotating tube. They demonstrated that when the tube rotates counterclockwise, the liquid film on the left side of the

tube becomes thinner compared to that of the right side.

Qiu et al. [46] simulated water and ethylene glycol falling films around a horizontal tube using a 3-D transient solver and the VOF method. They showed that the liquid viscosity is an important parameter affecting the falling film characteristics. The liquids with higher viscosity that spread over the tube surface are not able to form crests between adjacent liquid columns, and instead form an inline column flow.

Zhang et al. [47] investigated the effects of inlet liquid Reynolds number on the falling liquid film thickness by employing the VOF approach. Increasing the liquid Reynolds number increased the velocity and thickness of the liquid film. They observed that tube spacing had no effect on the film thickness at lower liquid Reynolds numbers.

Zhao et al. [48] numerically investigated liquid flow patterns on a horizontal tube by varying the inlet mass flow rate, tube diameter, and distribution height using a VOF method. Proposing a correlation for the film thickness, they observed that the minimum film thickness occurred at angles ranging from 110 to 150 degrees. Additionally, they found that the flow field near the two stagnation points was significantly influenced by changes in these operating conditions.

Han et al. [49] conducted a numerical study on the flow characteristics of a liquid film over three in-line horizontal tubes. They employed the VOF method and ANSYS Fluent for their simulations. They reported that under tilt conditions, the column mode transition to a sheet mode will occur. They also observed that, under tilt conditions, the average film thickness was greater on the upper perimeter of the tubes compared to the lower perimeter. This phenomenon was not observed under regular horizontal (non-tilt) conditions.

Wang et al. [3] employed a 3-D VOF model to investigate the flow of falling film in column mode using water and seawater liquid films. They observed that the falling film over a horizontal tube in column flow demonstrates robust 3-D characteristics and can be classified into five distinct regions. Additionally, they found that, within a stable region, both fluids exhibited similar film thickness.

Kumar-Poddar and Singh [50] compared results obtained from a VOF method with those from an Eulerian multiphase model for simulating the liquid-gas interface in a two-dimensional domain. They observed that both techniques exhibited similar trends in predicting film thickness. However, they did not provide enough information regarding the code and the Eulerian model used in their simulations. Additionally, they investigated the effects of varying liquid Reynolds number and tube diameter on the distribution of film thickness.

Tahir et al. [51] investigated the influence of gas flow rate on liquid film characteristics. They concluded that increasing the vapour velocity reduces the film thickness. Additionally, they observed that increasing the inlet liquid mass flow rate causes a slight downward shift in the location of the minimum film thickness. While a thinner liquid film can enhance heat transfer, they noted that for certain liquid Reynolds numbers, increasing the vapour velocity can lead to film disruption, which negatively impacts the heat transfer coefficient.

Zhou et al. [52] conducted research on the effects of various parameters on the distribution of liquid film thickness over a horizontal tube surface. A VOF method was applied in the simulations. The results indicate that increasing the gas flow velocity has a more noticeable effect on reducing the film thickness in the upper part of the tube. Similarly, increasing the tube diameter decreases the film thickness. Increasing the tube spacing at small tube diameters increases the thickness; however, it does not change the film thickness significantly at larger tube diameters. Also, increasing the liquid Reynolds number increases the film thickness. They indicated that precautions should be taken to prevent film disturbance and the formation of dry spots, as these can deteriorate heat transfer in the system.

The operating conditions and the quantities studied in the previous numerical works for a falling film on a horizontal tube under adiabatic conditions are presented in Table 1.2

The heat transfer characteristics of a falling film over horizontal tubes were numerically investigated by scholars, who mainly reported the local and average heat transfer coefficients in their work. Kocamustafaogullari and Chen [53] used a semi-analytical method to study the effects of

Table 1.2: Summary of numerical studies on the flow hydrodynamics over adiabatic horizontal tubes.

Author(s)	Year	Liquid film ^a	Setup ^b	Code ^c	TA ^d	Parameters Studied ^e
Sun et al. [39]	2012	W	2-D, L, Tr	F	1	$Re_{L,in}$, DH
Qiu et al. [40]	2015	W	2-D, L, S	F	2I	D
Qiu et al. [41]	2015	W	2-D, L, S	F	2I	$Re_{L,in}$
Hassan et al. [42]	2015	W	2-D, L, S	F	2I	TS
Li et al. [43]	2016	W/EG	3-D, T, Tr	F	2I	$Re_{L,in}$, $U_{G,in}$
Han et al. [44]	2017	W	2-D, L, Tr	F	1	TA
Lin et al. [45]	2018	W	2-D, L, S	ns	1	RS
Qiu et al. [46]	2018	W/EG	3-D, L, Tr	F	1	$Re_{L,in}$
Zhang et al. [47]	2018	W	3-D, L, Tr	F	1	$Re_{L,in}$, TS
Zhao et al. [48]	2018	W/SW	2-D, L, Tr	F	1	$Re_{L,in}$, D , DH, $T_{L,in}$
Han et al. [49]	2019	W	3-D, L, Tr	F	3I	$Re_{L,in}$, TS, TA
Wang et al. [3]	2019	W/SW	3-D, L, Tr	F	2I	$Re_{L,in}$, TS
Kumar-Poddar and Singh [50]	2021	W	2-D, L, Tr	ns	2I	$Re_{L,in}$, D
Tahir et al. [51]	2021	W	2-D, L, Tr	F	1	$Re_{L,in}$, $U_{G,in}$
Zhou et al. [52]	2023	W	2-D, T, Tr	ns	1	$Re_{L,in}$, $T_{L,in}$, $U_{G,in}$, D

^a Liquid film; W: Water, SW: Seawater, EG: Ethylene Glycol^b Setup; L: Laminar, T: Turbulent, S: Steady, Tr: Transient^c Code; F: ANSYS Fluent, ns: not specified^d TA (Tube Arrangement); 1: Single tube, 2I: Two in-line tubes, 3I: Three in-line tubes^e Parameters; DH: Distribution Height, TS: Tube Spacing, TA: Tilt Angle, RS: Rotational Speed

the Prandtl number, Reynolds number, and tube spacing on the film thickness of the flow over a horizontal tube. The tube wall boundary condition was either uniform heat flux or uniform temperature. They found that, at high liquid mass flow rates, the maximum film thickness is located at the

top half of the tube, and it moves towards the bottom as the liquid mass flow rate decreases. They also reported a decreasing trend for the local heat transfer coefficient along the tube circumferential angle.

Bourouni et al. [54] studied the heat transfer of the stagnation region using a boundary layer approach. They used pure water as working fluid and found that the local heat transfer coefficient is maximum in the impingement region at the top of the tube.

Hu et al. [55] numerically studied the flow and thermal characteristics of a water falling film using ANSYS Fluent. Their results indicate that the heat transfer coefficient increases by increasing the liquid mass flow rate, tube diameter, and evaporation temperature.

Yang et al. [56] studied the effects of inlet liquid Reynolds number and evaporation temperature variations on the film thickness and heat transfer coefficient. The film thickness was calculated using correlations presented by Chyu and Bergles [57]. They demonstrated that the local film thickness reaches a minimum value at a 90° angle, where local heat transfer is enhanced due to lower thermal resistance.

Yang et al. [58] conducted a numerical study using the VOF method on the effects of Reynolds number variation on the heat transfer coefficients and temperature of the falling film over a horizontal tube. Pure water was used as the liquid falling film. They found that convective heat transfer became dominant at higher Reynolds numbers.

Qi et al. [59] performed numerical and experimental studies on the liquid film flowing outside of an elliptical tube surface. They employed a VOF method along with $k - \epsilon$ turbulence model and selected seawater as working fluid. Their results revealed that for an elliptical tube case, the heat transfer coefficient can increase up to 20% compared with a circular tube.

Karmakar and Acharya [60] studied the impacts of different flow modes on the local and average heat transfer coefficient. They applied a 3-D model in their simulations using OpenFOAM and employed water, ethylene glycol, and their mixture as working fluids. The interface was modeled based on a VOF approach. They reported that in sheet flow mode, the highest circumferential vari-

ation of heat transfer coefficient around the tube was observed, while in the axial direction, the heat transfer coefficient was nearly uniform. The highest heat transfer coefficient was consistently observed in the impingement region for all flow modes. Also, they noted an increase in heat transfer coefficient while the tube spacing increased and as the tube diameter decreased.

Wunder et al. [61] analyzed condensation and evaporation processes of pure water inside and outside of a horizontal tube, respectively. They used a various combination of tube diameters and lengths and found that the heat transfer increased with tube diameter. They also found that the wall temperature change did not have a significant effect on the heat transfer coefficient.

Zhao et al. [62] utilized a VOF approach to explore the impacts of surface heat flux and liquid flow rate on the heat transfer coefficient of falling film over a horizontal tube. They revealed that the heat transfer coefficient increased with liquid flow rate. They also observed that changing the surface heat flux had a negligible effect on the average heat transfer coefficient.

Ning et al. [63, 64] used a 3-D model and VOF approach to investigate the effects of oil concentration and tube diameter on the heat transfer fluctuations. They observed that the fluctuations increase with oil mass fraction due to increased liquid viscosity. They also observed a non-linear increase in heat transfer coefficient with tube diameter due to an increasing impingement region.

Tahir et al. [65] performed an analysis of a heat transfer falling film on a horizontal tube by varying inlet liquid Reynolds number using the VOF method. They showed that a recirculation zone created in the liquid film enhances the heat transfer in the system. Additionally, they found that the heat transfer coefficient was improved at higher inlet temperatures due to a thinner liquid film, stronger recirculation, and a larger thermal developing region.

Wan et al. [66] conducted research on seawater liquid film over a single horizontal tube using Fluent. Their results indicate that film thickness increased with inlet liquid Reynolds number and salinity; however, it decreased with increasing the tube ellipticity. They reported that the heat transfer coefficient can be improved by increasing the Reynolds number, inlet temperature, and tube ellipticity. On the other hand, increasing the salt mass fraction in the liquid film caused a

heat transfer coefficient reduction. They also developed a correlation for the average heat transfer coefficient of seawater film over elliptical horizontal tubes.

Zhang and Zhou [67] utilized a VOF method to analyze the influence of tube shape on the flow and thermal characteristics of water film over a horizontal tube. They compared the results of a circular tube with oval tubes with different geometrical parameters. Their findings demonstrate that increasing the ovality reduces the film thickness, thereby enhancing heat transfer in the system. Table 1.3 summarizes the numerical studies of heat transfer over horizontal tubes.

Previous numerical studies discussed so far, are limited to those who only considered convective heat transfer and neglected mass transfer and phase change in their work. In case of evaporation occurs in the system, latent heat is transferred through the interface, and mass transfer occurs simultaneously. Al-Ansari and Owen [70] applied a semi-analytical approach to study the thermal and flow characteristics of the evaporation process around a horizontal tube and the condensation process inside the horizontal tube. Using a brine falling film, they concluded that a thicker film thickness could negatively affect the evaporation rate. Moreover, they noted the existence of a minimum film thickness limitation to prevent surface dryness.

Kouhikamali et al. [71] performed a numerical study on the effects of different tube arrangements on the heat transfer of tube bundle using a VOF method. They showed that that increasing the vertical spacing between tubes leads to a thinner falling film on lower tubes, thereby increasing the heat transfer coefficient. Additionally, a higher temperature difference between the wall and the inlet results in an increase in heat transfer coefficient and vaporization rate.

Bigham et al. [72] investigated pure water falling film evaporation on a horizontal tube bundle. They utilized a finite volume method based on the SIMPLE algorithm plus a VOF approach in an in-house code. A non-orthogonal grid was applied to solve the elliptic governing equations, including continuity, momentum, and energy equations. They studied the effects of inlet mass flow rate and temperature difference on the heat transfer coefficient and showed that the average heat transfer coefficient increases by enhancing the inlet mass flow rate. They also indicated that the

Table 1.3: Summary of numerical studies on the heat transfer over horizontal tubes.

Author(s)	Year	Liquid film ^a	Setup ^{b,c}	Code ^d	TA ^e	Wall B.C. ^f	Parameters Studied ^g
Kocamustafao-gullari and Chen. [53]	1988	W	2-D, T, S, SA	I	1	UWT/UHF	$Re_{L,in}$, TS
Bourouni et al. [68]	2001	W	2-D, L/T, S, BL	I	1	UWT	$Re_{L,in}$, $T_{L,in}$
Hu et al. [55]	2012	W	2-D, L, S	F	1	UWT	$Re_{L,in}$, D , $T_{L,in}$
Yang et al. [56]	2013	W	2-D, L, CE	ns	1	UWT	$Re_{L,in}$, $T_{L,in}$
Yang et al. [58]	2016	W	2-D, L/T, Tr	F	2I	UWT	$Re_{L,in}$
Qi et al. [59]	2016	SW	3-D, T, Tr	F	1	UWT	TSH
Karmakar and Acharya [60]	2017	W/EG	3-D, L, Tr	O	3I	UHF	$Re_{L,in}$, D , TS
Wunder et al. [61]	2017	SW	2-D/3-D, L, S, SA	I	1	UWT	TL, D
Zhao et al. [62]	2018	W/SW	2-D, L, Tr	F	1	UHF	$Re_{L,in}$, D , DH, $T_{L,in}$, q''_{wall}
Hao et al. [69]	2019	W and G	3-D, L	ns	1	UHF	$Re_{L,in}$, D , q''_{wall}
Ning et al. [64]	2020	OS	3-D, T, Tr	F	1	UHF	$Re_{L,in}$, D
Ning et al. [63]	2020	OS	3-D, T, Tr	F	1	UHF	$Re_{L,in}$, D
Tahir et al. [65]	2021	W	2-D, L, Tr	F	1	UWT	$Re_{L,in}$, $T_{L,in}$
Wan et al. [66]	2021	SAL	2-D, L, Tr	F	1	UHF	$Re_{L,in}$, $T_{L,in}$, S, D , TSH
Zhang and Zhou [67]	2022	W	2-D, L, Tr	F	1	UHF	$Re_{L,in}$, TSH

^a Liquid film; W: Water, SW: Seawater, EG: Ethylene Glycol, G: Glycerin, OS: Oily Sewage, SAL: Saline Water

^b Setup; L: Laminar, T: Turbulent, S: Steady, Tr: Transient

^c All studies used a VOF method except those noted with SA: Semi-Analytical, BL: Boundary Layer, and CE: Correlation Equations

^d Code; I: In-house, F: Fluent, O: OpenFOAM, ns: not specified

^e TA (Tube Arrangement); 1: Single tube, 2I: Two in-line tubes, 3I: Three in-line tubes

^f B.C. (Boundary Condition); UWT: Uniform Wall Temperature, UHF: Uniform Heat Flux

^g DH: Distribution Height, TS: Tube Spacing, TSH: Tube Shape, S: Salinity, TL: Tube Length

net vapour production decreased by increasing the liquid inlet mass flow rate.

Abraham and Mani [73] performed a numerical study on the heat and mass transfer of the falling film evaporation over a horizontal tube. They used ANSYS Fluent with a VOF approach. They studied the effects of surface temperature and tube diameter on the local heat transfer coefficient and concluded that the heat transfer coefficient decreases after the impingement region. Increasing the liquid inlet Reynolds number up to a certain value, improved convective heat transfer which increased the heat transfer coefficient. For higher liquid Reynolds numbers, however, the heat transfer coefficient did not change due to the increase of the film thickness. They showed that the increase of the inlet liquid Reynolds number beyond 750 negatively affected heat transfer and evaporation rate. Also, an increase in the tube diameter reduced the heat transfer coefficient.

Lin et al. [74] used a 3-D VOF approach to model flow over a horizontal tube. They used pure water as the working fluid and determined the effects of the tube diameter and liquid Reynolds number on the film thickness and heat transfer coefficient.

Balaji et al. [75] numerically studied the effect of tube geometry and liquid feeder height on the heat transfer of falling film evaporation over a horizontal tube. They used a 2-D solution of the elliptic governing equations and a VOF approach. The liquid falling film was either pure or saline water in their study. They studied the effects of changes in the tube diameter and liquid feeder height on the heat transfer coefficient. Their results indicated that seawater properties diminish the heat transfer coefficient compared to freshwater, but do not significantly affect the film thickness.

Balaji et al. [76] extended their research in [75] by the same numerical methodology to predict the water liquid film thickness around the tube. They observed that the minimum liquid film thickness is located between 85° and 127° , and that the fully developed thermal region extends with the increase of the feeder height and heat flux.

There are other numerical studies that investigated other parameters such as surface tension or non-condensable gas desorption of liquid falling film over a horizontal tube [77, 78]. These and other studies are discussed in notable open literature reviews of liquid falling film over horizontal

Table 1.4: Summary of numerical studies on evaporation over horizontal tubes.

Author(s)	Year	Liquid film ^a	Setup ^{b,c}	Code ^d	MTM ^e	TA ^f	Wall B.C. ^g	Parameters Studied ^h
Al-Ansari and Oven [70]	1999	B	2-D/3-D, L/T, S, SA	I	ns	1	UWT	$Re_{L,in}$
Kouhikamali et al. [71]	2014	W	2-D, T, Tr	I	Lee	TB	UWT	$T_{L,in}, T_{wall}$
Bigham et al. [72]	2015	W	2-D, T, S	I	Lee	2I	UWT	$Re_{L,in}$
Abraham and Mani [73]	2015	W/SW	2-D, T, Tr	F	ns	1/TB	UWT	$Re_{L,in}, D$
Lin et al. [74]	2019	W	3-D, L, Tr	F	Lee	1	UHF	$Re_{L,in}, D$
Balaji et al. [75]	2019	W/SW	2-D, L, Tr	F	Lee	2I	UWT	$Re_{L,in}, DH, D$
Balaji et al. [76]	2020	W	2-D, L, Tr	F	Lee	2I	UHF	$Re_{L,in}, DH, q''_{wall}$

^a Liquid film; B: Brine, W: Water, SW: Seawater

^b Setup; L: Laminar, T: Turbulent, S: Steady, Tr: Transient

^c All studies used a VOF method except the one noted with SA: Semi-Analytical

^d Code; I: In-house, F: Fluent, ns: not specified

^e MTM (Mass Transfer Model); Lee: Lee model, ns: not specified

^f TA (Tube Arrangement); 1: Single tube, 2I: Two in-line tubes, 3I: Three in-line tubes, TB: Tube Bundle

^g B.C. (Boundary Condition); UWT: Uniform Wall Temperature, UHF: Uniform Heat Flux

^h Parameters; DH: Distribution Height

tube surface [79–82]. Table 1.4 summarizes the numerical studies of evaporation over horizontal tubes. It is noted that all of the previous models that solved the full governing equations (elliptic approach) applied a volume of fluid (VOF) to determine the location of the liquid and gas interface. As shown in Table 1.4, previous numerical studies mostly used the Lee mass transfer model in their simulations. This model is implemented in commercial software like Fluent and is widely used for modeling phase-change processes; however, it relies on empirical coefficients that depend on the working fluid and flow conditions. There are also other studies in the literature that utilize empirical

equations or theoretical analyses [83,84] to calculate the mass transfer at the interface using Fluent. Therefore, it would be a significant advance to implement a mass transfer model for the simulation of the evaporation process that is not restricted by correlations and approximations. In the present study, a sharp interface model is used that determines the evaporation rate using an energy balance at the interface. The interface location can also be calculated using a mass balance analysis at each liquid column in the domain, which has the advantage of precisely predicting the interface location, unlike methods such as VOF that are not capable of determining it accurately. To the best of the author's knowledge, the implementation of a sharp interface model in the simulation of the desalination process over a horizontal tube has not been previously addressed.

1.3.2 Experimental Studies

1.3.2.1 Experimental Studies: Vertical Channel and Plate Geometries

There are relatively few experimental studies in this category because of difficulties in measurement inside a channel. Tsay et al. [15] conducted an experimental study to investigate the evaporation characteristics for a single vertical plate. A preheater was used to heat the liquid ethanol film falling down the plate. The wall temperature distribution and a total temperature drop of the liquid for different liquid mass flow rates were reported in this study.

Yan et al. [1] studied the evaporation of falling liquid film through interfacial heat and mass transfer in a vertical channel. They measured the wall temperature and heat and mass transfer rates for wide variety of values of the inlet temperature, channel width, and liquid mass flow rate for water and ethanol. They showed that the cooling rate of the liquid film due to the evaporative latent heat transfer depends mainly on the inlet liquid temperature and liquid mass flow rate.

Tsay and Lin [16] performed a study to measure the heat transfer coefficient for a single plate for different thermal conditions, inlet liquid mass flow rates, and gas stream velocities. Also, they proposed a new correlation of the Nusselt number for heat transfer from the wall to the liquid film.

Table 1.5: Review of experimental studies over plates or inside channels.

Author(s)	Year	Liquid film	Wall B.C. ^a	$T_{L,in}$ [°C]	$T_{G,in}$ [°C]	$\dot{m}_{L,in}$ [kg/m · s]
Tsay et al. [15]	1990	ethanol	A	30 – 35	30	0.01 – 0.04
Yan et al. [1]	1991	water ethanol	A	27 – 60	30 – 31	0.01 – 0.04
Tsay and Lin [16]	1995	water	UHF	30 – 50	30	0.02 – 0.04

^a B.C. (Boundary Condition); A: Adiabatic, UHF: Uniform Heat Flux

Table 1.5 summarizes the relevant experimental studies of evaporation inside vertical channels. The inlet pressure is equal to the atmospheric pressure in all studies summarized in this table. Among the studies listed in the table, the experimental data presented by Yan et al. [1] have been widely used by scholars for validation purposes, so the results of the present study are compared with those provided by Yan et al. [1].

1.3.2.2 Experimental Studies: Horizontal tube Geometry

The falling film flow over a horizontal tube has been investigated by some researchers who primarily study the effects of varying parameters on the film thickness or heat transfer coefficient. There are two main methods for measuring falling film thickness: intrusive and non-intrusive. The conducting probe method is an example of an intrusive method in which the probe can affect the liquid film distribution. When the probe touches the liquid, there is a chance that the liquid climbs along the probe due to surface tension, which affects the accuracy of the measurements. In non-intrusive techniques like the laser-induced fluorescence method, accuracy is not affected by any external instrument and mainly depends on the image resolution and number of pixels. For measuring the heat transfer coefficient, the surface temperature is recorded using thermocouples embedded into the tube surface.

Fletcher et al. [85] studied the effects of different parameters on the evaporation of seawater falling film over a horizontal tube. The liquid, maintained at its saturation temperature, enters the system through a perforated plate. Electric power was applied to have a constant heat flux at the tube surface. The temperature of the liquid film was continuously monitored to ensure a steady-state condition. They reported that, at the highest heat flux, the evaporated liquid was less than two percent of the feed water, resulting in negligible change in the salinity of the liquid film along the tube surface. They also concluded that the heat transfer coefficient is higher for smaller diameter.

Chyu and Bergles [57] studied the evaporation of pure water film falling over a horizontal heated tube used in an ocean thermal energy conversion (OTEC) system. A saturated liquid falling film was introduced on a tube surface through a slot. The liquid flow rate at the inlet was measured using a rotameter. Six thermocouples were installed on the tube surface to measure the wall temperature, with the average wall temperature calculated from these six measurements. Because the wall was sufficiently thick, the tube surface was considered to be at a constant temperature. They investigated the effects of liquid film mass flow rate and liquid feed height on the heat transfer coefficient. They observed that the heat transfer coefficient was less sensitive to the variation of

liquid feed height at low liquid Reynolds numbers. The variation in feed height also had a negligible impact on the heat transfer coefficient at high heat fluxes due to the nucleate boiling in the film that controlled the hydrodynamics of the flow.

Parken et al. [86] investigated the local and average heat transfer coefficient over a single horizontal tube surface. The pure water falling film entering the system was either saturated or subcooled. They employed both a perforated plate and a thin-slot water distribution system in their study. They reported that the thin-slot water distribution system can be more accurately controlled. On the other hand, a perforated plate provided a thinner boundary layer under similar conditions, thereby leading to a higher heat transfer coefficient in the system. Eight thermocouples were utilized to record the wall temperature. The liquid film thickness was visualized through Pyrex windows surrounding the measurement section, and images were captured to record the occurrence of nucleate boiling. They observed nucleate boiling in the liquid film for subcooling levels less than 6°C. Also, they found that subcooling within the range of 6°C to 55°C did not significantly affect the heat transfer coefficient.

Hu and Jacobi [87] investigated liquid falling film characteristics of four different working fluids flowing over two in-line horizontal adiabatic tubes. The test section was constructed of transparent plastic to visualize the film modes. They studied different flow modes ranging from droplet to sheet for different fluids. The tests were conducted either in a quiescent surrounding or in the presence of a co-current air flow. They observed that in the presence of air flow, the transitional Reynolds number from droplet to column increased about 25%. Hu and Jacobi [4] also used a setup similar to [87] to study the impacts of different flow modes on the sensible heat transfer of a liquid falling film over two horizontal tubes. They measured the surface temperature using 24 thermocouples. They reported both local and average heat transfer coefficients for various liquid Reynolds numbers and different working fluids.

Fujita and Tsutsui [88] studied evaporative heat transfer of liquid falling films over horizontal tubes using Freon-11 as the working fluid. They used copper tubes and electrical heaters to obtain a

uniform wall heat flux. They showed that, for heat flux levels lower than that for boiling initiation, the heat transfer coefficients of evaporating films are independent of the heat flux.

Gstoehl et al. [89] used an experimental method to measure the film thickness over a horizontal tube using either water or ethylene glycol liquid film. The liquid film was visualized using the laser-induced fluorescent method, where a laser sheet illuminated the film over the tube surface, making the free surface visible due to light interaction with the liquid. Subsequently, a digital high-speed camera was used to capture images from the film surface. They compared their results against Nusselt falling film theory results and concluded that the Nusselt theory reasonably predicts the film thickness on the top of the tube; however, it considerably overestimates the film thickness on the lower perimeter.

Yang and Shen [90] studied evaporation for seawater and examined the effects of inlet liquid mass flow rate and the distributor height on the average heat transfer coefficient. Four thermocouples were embedded into the tube surface to measure the temperature. They observed that the heat transfer coefficient increased by increasing the distributor height and liquid mass flow rate. There was a slight difference between the heat transfer coefficients for pure water and saline water.

Hou et al. [91] experimentally investigated the liquid falling film of pure water or seawater over horizontal tubes. A flow distribution system was employed to provide a uniform flow over the tube surface. To measure the liquid film, they utilized a displacement micrometer that treated the liquid and air as electric and dielectric media, respectively. A probe was used to detect the liquid-gas interface. This device was connected to an electric circuit that displayed varying voltage outputs. When the probe was exposed to air, the electric circuit recorded a low voltage. Conversely, it registered a high voltage when the probe contacted the liquid. This method was effective at detecting the liquid-gas interface. They concluded that the intertube spacing and the film Reynolds number are the main factors affecting the liquid film distribution. They also found that the tube diameter did not have an impact on the film thickness.

Mu et al. [92] conducted an experimental study to examine the impacts of liquid Reynolds

number, surface heat flux, and inlet temperature on the heat transfer coefficient for various fluids. Their results showed that the local heat transfer coefficient decreased along the tube surface initially but increased towards the lower part of the tube. Furthermore, they identified the maximum film flow rate at which the highest heat transfer coefficient was achieved. They concluded that, when the liquid mass flow rate is beyond a certain value, there is not a significant change in the average heat transfer coefficient with increase of the mass flow rate.

Chen et al. [2] experimentally investigated the effects of the properties of pure and saline water on the film thickness around a horizontal tube. They utilized a laser-induced fluorescence technique to measure the falling film thickness. The fluorescent was induced in the liquid by the laser, and images of the liquid-gas interface were captured using a digital camera. They demonstrated that under similar working conditions, the heat transfer coefficient of seawater is lower than that of freshwater. They also concluded that the saline water film thickness is thicker than that of pure water due to higher surface tension and viscosity.

Narvez-Romo and Simes-Moreira [93] investigated the heat transfer and the thickness of falling liquid water film over heated horizontal tubes. Flows with gas phase Reynolds numbers up to 940 were examined in both sub-cooled and saturated liquid regimes. An intrusive method was used for measuring the film thickness. An electronic circuit was utilized to detect electrical continuity between the probe tip and the liquid film. When the probe contacted the liquid film, the electrical circuit closed, and the interface location was recorded by a micrometer reading. They observed that the local heat transfer coefficient was always highest at the horizontal tube top region. Based on the experimental data, they proposed a new Nusselt number correlation that is a function of liquid Reynolds number and Prandtl number.

Shen et al. [5] conducted research on the heat transfer process in a horizontal tube seawater falling film evaporator. An internal electric heater was employed to maintain a uniform heat flux at the tube surface, and several thermocouples were used to measure the surface temperature. They demonstrated that the average heat transfer coefficient decreases with increasing salinity and

remains independent of the wall heat flux.

Recently, Li et al. [94] conducted experimental research on falling film evaporation using both fresh water and seawater. They investigated the effects of inlet Reynolds number, tube spacing, and salinity on the heat transfer coefficient. Their findings showed that the heat transfer coefficient of seawater is lower than that of pure water under similar conditions. Additionally, they developed a correlation for the Nusselt number valid for liquid Reynolds numbers ranging from 118 to 1979.

Table 1.6 summarizes the relevant experimental studies of evaporation over horizontal tubes. The number of experimental studies that can be used for the validation of the results presented in this work is limited. In some studies, the provided information is not sufficient for a precise comparison, or the liquid falling film is turbulent. The results from the present elliptic model are compared with the experimental data presented by Chen et al. [2], Hu and Jacobi [4], and Shen et al. [5] in Chapter 8.

1.4 Contributions of the present work

The two-phase fluid flow and heat and mass transfer characteristics of the evaporation phenomenon are complicated. The governing equations have strong non-linear and inter-equation coupling effects plus heat and mass transfer are strongly inter-dependent, so a robust numerical solution approach is needed. Some of previous studies simplified the solution by using the boundary layer approximations and a marching scheme. That approach is not capable of modelling reverse flows and recirculation zones that will occur due to buoyancy effects and flow around a tube. All of the previous models that solved the full governing equations (elliptic approach) applied a volume of fluid (VOF) method which solved an additional equation for the gas volume fraction. The main disadvantage of this approach is that it is not able to determine accurately the location of the liquid and gas interface. Therefore, it cannot accurately apply the interface jump conditions. It is concluded that, although previous numerical studies have investigated the heat and flow characteristics

Table 1.6: Summary of experimental studies of liquid falling film over horizontal tubes.

Author(s)	Year	Liquid film ^a	Mass transfer ^b	Tube Number	Tube Diameter [mm]	Tube Spacing [mm]	Surface B.C. ^c	Parameters Studied ^d
Fletcher et al. [85]	1975	SW	Y	1	25.4-50.8	–	UHF	$Re_{L,in}$, D , q''_{wall} , $T_{L,in}$
Chyu and Bergles [57]	1987	W	Y	1	25.4	–	UWT	$Re_{L,in}$, DH, T_{wall}
Parken et al. [86]	1990	W	Y	1	25.4-50.8	–	UHF	$Re_{L,in}$, q''_{wall} , $T_{L,in}$
Hu and Jacobi [87]	1996	W/O/EG/A	N	2	9.5-22.2	5-50	A	$Re_{L,in}$, TS
Hu and Jacobi [4]	1996	W/EG	N	2	15.8-22.2	5-50	UHF	$Re_{L,in}$
Fujita and Tsutsui [88]	1998	F	Y	1	25	–	UWT	$Re_{L,in}$, q''_{wall} , DH
Gstoehl et al. [89]	2004	W/EG	N	3	19.05	3.2-19.4	UWT	$Re_{L,in}$, TS
Yang and Shen [90]	2008	W/SW	Y	2	14	7	UWT	$Re_{L,in}$, DH
Hou et al. [91]	2012	W/SW	N	3	20-32	10-40	A	D , TS
Mu et al. [92]	2014	W/SW	Y	2	25.4	31.6	UHF	$Re_{L,in}$, q''_{wall} , $T_{L,in}$
Chen et al. [2]	2015	W/SW	N	2	19-25.4	20-40	A	$Re_{L,in}$, D , TS
Narvez-Romo and Simes-Moreira [93]	2017	W	Y	1	19	–	UHF	$Re_{L,in}$, $T_{L,in}$
Shen et al. [5]	2017	SW	Y	2	19-25.4	15.2-31.7	UHF	$Re_{L,in}$, D , TS
Li et al. [94]	2024	W/SW	Y	2	19-38	5.7-47.5	UHF	$Re_{L,in}$, $T_{L,in}$, TS

^a Liquid film; SW: Seawater, W: Water, O: Oil, EG: Ethylene Glycol, A: Alcohol, F: Freon-11

^b Mass transfer: Y:Yes, N:No

^c B.C. (Boundary Condition); UHF: Uniform Heat Flux, UWT: Uniform wall Temperature, A: Adiabatic

^d Parameters; TS: Tube Spacing, DH: Distributor Height

of the evaporation process, using a full elliptic model with an accurate method for determination of the liquid-gas interface is lacking. The aim of this research is to utilize an elliptic approach with an interface tracking method for the heat and mass transfer simulation. This approach not only provides the opportunity to study complex cases with reversal flow and recirculation zones, but also uses an accurate representation of the liquid-gas interface, and the coupled heat and mass condition there.

The present study comprises four steps. In each step, the numerical model was developed based on the desired working conditions.

1. Parabolic Pure Water Channel Model: In the first step, a complete parabolic laminar two-phase flow model is developed to simulate the evaporation from a liquid falling film into a co-current gas mixture based on the conservation of momentum, mass, and energy. Fundamental balances of energy, mass, and shear force at the interface assured the proper interaction between the liquid and mixture phases. The solution fields included the axial velocity, transverse mass flux, and temperature for both phases plus the air mass fraction, the film thickness, and the axial pressure gradient.

2. Elliptic Pure Water Channel Model: In the second step, the numerical model utilizes an elliptic approach to study the laminar two-phase flow phenomenon of the evaporation of pure water falling film into a co-current gas mixture. The equations for mass, momentum, gas mass fraction, and energy are solved on a co-located structured non-orthogonal grid for both the liquid and gas phases. The solution field variables, including the axial velocity, transverse velocity, pressure, and temperature for both phases, plus the air mass fraction for the gas phase were solved simultaneously in the entire domain. Once all solution variables are computed on a fixed grid, the interface location is sharply determined by imposing mass balance at the end of each time step for all liquid columns within the domain. This precise interface resolution enables more accurate determinations of the interface location, interfacial shear stress, and velocity profiles compared to methods such as VOF, where the interface is estimated in control volumes by varying the volume fractions from zero to

one. The iterative procedure continues until a steady state solution convergence is obtained. The excess moisture condensation (EMC) model was also introduced as a novel method to address supersaturation in the system.

3. Elliptic Salt water Channel Model: In the third step, the elliptic model is developed to study the flow and thermal characteristics of the evaporation process of seawater inside a vertical parallel plate channel. To the best knowledge of the author, the implementation of an elliptic approach to a two-phase falling film desalination process inside a vertical parallel plate channel has not been previously addressed. Therefore, the present numerical model is used investigate the effects of mixed convection and salt concentration on the flow and thermal characteristics of the evaporation process of liquid saline water film within a vertical parallel plate channel.

4. Elliptic Salt water Horizontal Tube Model: In the last step, the research is extended to model the evaporation of fresh water and salt water falling film over a horizontal tube. The elliptic approach which is capable of capturing the re-circulation zones is used for the simulations. To the best knowledge of the author, the elliptic model developed in the present study offers a more comprehensive and detailed approach compared to any previous numerical studies on falling film evaporation.

1.5 Layout of the Thesis

The remaining chapters of this thesis are organized as follows:

Chapter 2 presents the parabolic and elliptic mathematical models including the governing equations in both liquid and gas phases along with all the equations at the interface. The interface moving strategy is explained. The boundary conditions are described in detail in this chapter.

Chapter 3 presents the discretisation of the domain and grid generation for both parabolic and elliptic models. The transformed governing equations are given for the parabolic model. The basic nomenclature of the grid system is also illustrated.

Chapter 4 explains the numerical solution method in parabolic and elliptic models. In this chapter, discretisation of the governing equations is described. There is a detailed discussion of the each term in the set of equations, as well as the boundary conditions implementation.

Chapter 5 presents the results of the pure liquid parabolic model for the falling film evaporation inside a parallel plate vertical channel. This chapter includes the comparison of the results with previous studies and new results that investigate the effects of different parameters on the flow and thermal characteristics of the system.

Chapter 6 presents detailed results for the pure liquid elliptic model solution of evaporation inside a vertical parallel plate channel. The results include comparison with the parabolic model and a previous numerical study. The effects of buoyancy forces on the flow features and heat and mass transfer of the system are discussed.

Chapter 7 provides a comprehensive analysis of the elliptic model solution for evaporation of salt water within a vertical parallel plate channel. The basis of the evaporation model is validated for pure water falling film evaporation. The performance of this model is illustrated by studying the impacts of different parameters on the details of the flow and heat and mass transfer of a falling film thermal desalination system.

Chapter 8 presents the elliptic model results investigating salt water film flow around a horizontal tube in contact with a co-current gas stream. This chapter includes the validation results and also new results for the cases with different salinity, liquid mass flow rate, mixture Reynolds number, and gas mass fraction.

Chapter 9 provides a summary of the main results in this work and presents the significant conclusions.

Chapter 2

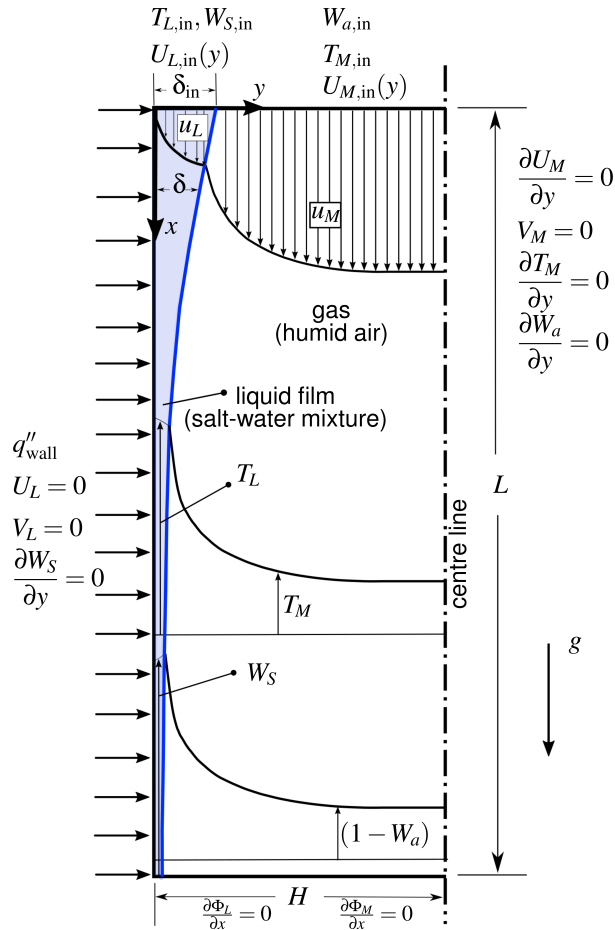
Mathematical Model

2.1 Introduction

In this study, the simultaneous heat and mass transfer processes involved in the evaporation of pure water and salt water are analyzed numerically using conservation laws applied to a domain of control volumes. Both liquid and gas phases are assumed to be laminar. The governing equations for describing the two-dimensional, incompressible, Newtonian fluid flows of the liquid and gas are derived based on the conservation of mass, momentum, and energy under a steady-state condition. The governing equations are expressed in Cartesian coordinates, x and y , where x represents the stream-wise direction, and y denotes the transverse (wall-normal) direction. It is assumed that the interface between the liquid and vapour is smooth, non-wavy, and impermeable to salt in the liquid and to air in the mixture, respectively. The liquid and gas phase equations are connected by interface conditions that are applied at the liquid-gas interface.

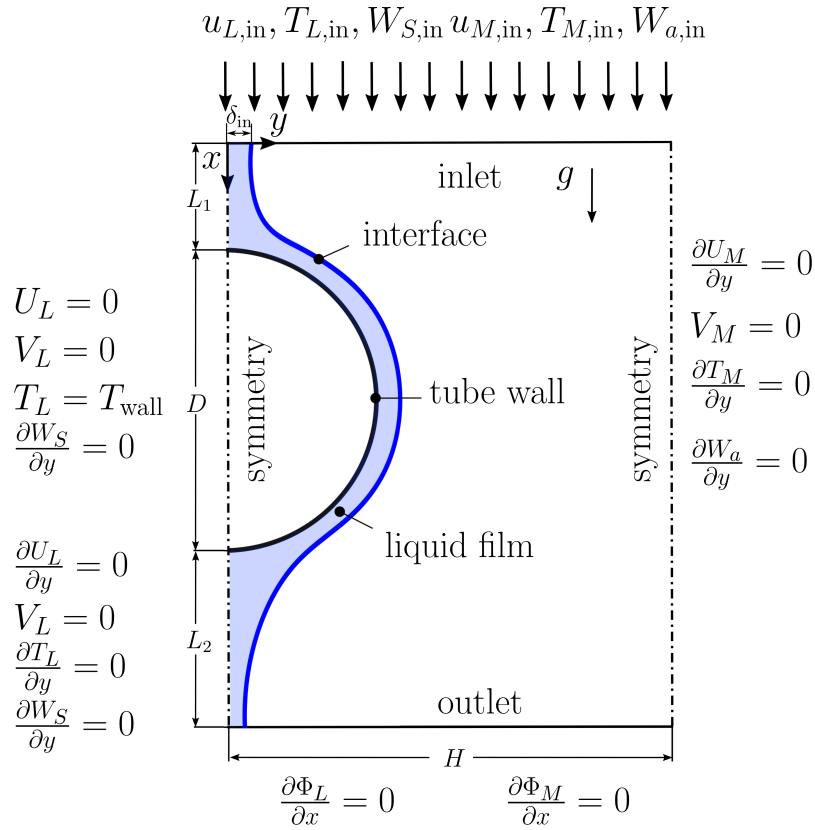
2.2 Problem Statement

A diagram of the physical model considered for the flow inside a parallel plate channel is shown in Fig. 2.1. A fully developed two-phase downward flow of a gas-vapour mixture and liquid enters a vertical channel with a channel half width of H and plate length L . The liquid film with uniform inlet temperature enters the channel with initial thickness of δ_{in} . The gas-vapour mixture enters with uniform temperature and gas mass fraction. The inlet axial velocity of both the film and mixture are specified by a fully developed profile; the transverse inlet velocities are zero. The liquid is flowing over the wall surface at which a constant heat flux is applied. Heat and mass transfer occur at the phase interface. The liquid film thickness decreases along the channel due



to mass removal. It is important to note that for the case of pure water evaporation, the salt mass fraction is equal to zero in all boundaries. The boundary conditions will be discussed in more detail with the set of governing equations shortly.

A diagram of the physical model of falling film over a horizontal tube is depicted in Figure 2.2. The liquid and gas phases enter the domain with uniform velocities and temperatures at the inlet boundary. The liquid film flows over the tube surface while evaporating to the gas phase. Due to the symmetry condition, only half of the physical problem is solved. The liquid film falling distances above the tube and below the tube are L_1 and L_2 , respectively, and H is the solution



2.3.1 Liquid Phase

The liquid phase mass, momentum, and energy conservation equations are:

- Liquid continuity equation

$$\frac{\partial(\rho_L U_L)}{\partial x} + \frac{\partial(\rho_L V_L)}{\partial y} = 0 \quad (2.1)$$

- Liquid momentum equation in the x direction

$$\frac{\partial(\rho_L U_L U_L)}{\partial x} + \frac{\partial(\rho_L V_L U_L)}{\partial y} = -\frac{dP}{dx} + \frac{\partial}{\partial y} \left(\mu_L \frac{\partial U_L}{\partial y} \right) + \rho_L g_x \quad (2.2)$$

- Liquid energy equation

$$\frac{\partial}{\partial x} (\rho_L U_L C_{p,L} T_L) + \frac{\partial}{\partial y} (\rho_L V_L C_{p,L} T_L) = \frac{\partial}{\partial y} \left(k_L \frac{\partial T_L}{\partial y} \right) \quad (2.3)$$

2.3.2 Gas Phase

The gas phase mass, momentum, and energy conservation equations are:

- Gas continuity equation

$$\frac{\partial(\rho_M U_M)}{\partial x} + \frac{\partial(\rho_M V_M)}{\partial y} = 0 \quad (2.4)$$

- Gas momentum equation in the x direction

$$\frac{\partial(\rho_M U_M U_M)}{\partial x} + \frac{\partial(\rho_M V_M U_M)}{\partial y} = -\frac{dP}{dx} + \frac{\partial}{\partial y} \left(\mu_M \frac{\partial U_M}{\partial y} \right) + \rho_M g_x \quad (2.5)$$

- Gas energy equation

$$\begin{aligned} \frac{\partial}{\partial x} (\rho_M U_M C_{p,M} T_M) + \frac{\partial}{\partial y} (\rho_M V_M C_{p,M} T_M) = \\ \frac{\partial}{\partial y} \left(k_M \frac{\partial T_M}{\partial y} \right) + \frac{\partial}{\partial y} \left(\rho_M D^{AB} (C_{p,g} - C_{p,v}) \frac{\partial W_a}{\partial y} T_M \right) \end{aligned} \quad (2.6)$$

- Gas mass fraction equation

$$\frac{\partial(\rho_M U_M W_a)}{\partial x} + \frac{\partial(\rho_M V_M W_a)}{\partial y} = \frac{\partial}{\partial y} \left(\rho_M D^{AB} \frac{\partial W_a}{\partial y} \right) \quad (2.7)$$

The pressure, P , in the governing equations is the local relative static pressure. To calculate the flow properties in the liquid and gas phases and the interface, a reference pressure of $P = P_{L,\text{in}}$ is added to the local pressure. The thermodynamic and transport properties are calculated based on the local temperature, mass fraction, and pressure using equations found in Siow [95].

The overall conservation of mass is represented as:

$$\int_0^\delta \rho_L U_L dy + \int_\delta^H \rho_M U_M dy = \dot{m}'_{L,\text{in}} + \dot{m}'_{M,\text{in}} \quad (2.8)$$

This equation is used to implicitly determine the pressure gradient, dP/dx , through coupling with the momentum equations.

2.3.3 Interface Conditions

The following conditions are applied at the phase interface:

- Continuity of velocity and shear stress

$$U_L = U_M, \quad \mu_L \frac{\partial U_L}{\partial y} = \mu_M \frac{\partial U_M}{\partial y} \quad (2.9)$$

- Continuity of mass flux

$$\rho_L V_L + \rho_L U_L \frac{\partial \delta}{\partial x} = \rho_M V_M + \rho_M U_M \frac{\partial \delta}{\partial x} = \dot{m}''_{\text{intf}} \quad (2.10)$$

- Continuity of the temperature

$$T_L = T_M = T_{\text{intf}} \quad (2.11)$$

Saturation is assumed at the interface. The interface temperature is equal to the saturation temperature corresponding to the partial pressure of the vapour at the interface ($P_{v,\text{intf}}$). Using the assumption of ideal gas mixture, the partial pressure of vapour is calculated as:

$$P_{v,\text{intf}} = \left(\frac{1 - W_{g,\text{intf}}}{1 + W_{g,\text{intf}} \left(\frac{M_v}{M_a} - 1 \right)} \right) P_{\text{intf}} \quad (2.12)$$

- Impermeability of gas at the interface

$$-\rho_M D^{AB} \left. \frac{\partial W_a}{\partial y} \right|_{M,\text{intf}} = \dot{m}''_{\text{intf}} W_a \quad (2.13)$$

- Continuity of energy

$$k_L \left. \frac{\partial T_L}{\partial y} \right|_{L,\text{intf}} = k_M \left. \frac{\partial T_M}{\partial y} \right|_{M,\text{intf}} - \dot{m}''_{\text{intf}} h_{fg} \quad (2.14)$$

In the coupled equation set, the interface energy balance equation is used to determine the film thickness, δ , implicitly.

2.3.4 Domain and Boundary Condition Definitions

The boundary conditions shown in Figure 2.1 are prescribed as follows:

- at the inlet ($x = 0$): uniform temperature and mass fraction and fully developed velocity profiles

$$T_L = T_{L,\text{in}}, \quad U_L = U_{L,\text{in}}(y), \quad V_{L,\text{in}} = 0 \quad \text{for} \quad 0 \leq y \leq \delta_{\text{in}} \quad (2.15)$$

$$T_M = T_{M,\text{in}}, \quad U_M = U_{M,\text{in}}(y), \quad V_{M,\text{in}} = 0 \quad W_a = W_{a,\text{in}} \quad \text{for} \quad \delta_{\text{in}} \leq y \leq H \quad (2.16)$$

$$P_{L,\text{in}} = P_{M,\text{in}} = P_{\text{in}} \quad (2.17)$$

For given film and gas Reynolds numbers, the equations presented in Appendix A are utilized to specify the inlet liquid and mixture velocity fully-developed profiles along with the corresponding film thickness and pressure gradient.

- at the wall beside the liquid phase ($y = 0$): constant heat flux, no slip and no penetration conditions at the wall

$$-k_L \frac{\partial T_L}{\partial y} = q''_{\text{wall}}, \quad U_L = 0, \quad V_L = 0 \quad (2.18)$$

- At the centre line ($y = H$)

$$\frac{\partial T_M}{\partial y} = 0, \quad \frac{\partial W_a}{\partial y} = 0, \quad \frac{\partial U_M}{\partial y} = 0, \quad V_M = 0 \quad (2.19)$$

This mathematical model, consisting of governing equations and boundary and interface conditions is used to determine the velocity and temperature in both phases, the air mass fraction in the gas phase, the film thickness, and the pressure gradient.

2.4 Elliptic Model Governing Equations

2.4.1 Liquid Phase

- Liquid continuity equation

$$\frac{\partial(\rho_L)}{\partial t} + \frac{\partial(\rho_L U_L)}{\partial x} + \frac{\partial(\rho_L V_L)}{\partial y} = 0 \quad (2.20)$$

- Liquid momentum equation in the x direction

$$\frac{\partial(\rho_L U_L)}{\partial t} + \frac{\partial(\rho_L U_L U_L)}{\partial x} + \frac{\partial(\rho_L V_L U_L)}{\partial y} = -\frac{\partial P_L}{\partial x} + \frac{\partial}{\partial x} \left(\mu_L \frac{\partial U_L}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_L \frac{\partial U_L}{\partial y} \right) + \rho_L g_x \quad (2.21)$$

- Liquid momentum equation in the y direction

$$\frac{\partial(\rho_L V_L)}{\partial t} + \frac{\partial(\rho_L U_L V_L)}{\partial x} + \frac{\partial(\rho_L V_L V_L)}{\partial y} = -\frac{\partial P_L}{\partial y} + \frac{\partial}{\partial x} \left(\mu_L \frac{\partial V_L}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_L \frac{\partial V_L}{\partial y} \right) + \rho_L g_y \quad (2.22)$$

- Liquid energy equation

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_L C_{p,L} T_L) + \frac{\partial}{\partial x} [\rho_L U_L (C_{p,L} T_L + W_S (\bar{h}_S - \bar{h}_W))] + \frac{\partial}{\partial y} [\rho_L V_L (C_{p,L} T_L + W_S (\bar{h}_S - \bar{h}_W))] = \\ \frac{\partial}{\partial x} \left(k_L \frac{\partial T_L}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_L \frac{\partial T_L}{\partial y} \right) + \frac{\partial}{\partial x} \left(\rho_L D_L^{AB} \frac{\partial W_S}{\partial x} (\bar{h}_S - \bar{h}_W) \right) + \frac{\partial}{\partial y} \left(\rho_L D_L^{AB} \frac{\partial W_S}{\partial y} (\bar{h}_S - \bar{h}_W) \right) \end{aligned} \quad (2.23)$$

- Liquid mass fraction equation

$$\frac{\partial(\rho_L W_S)}{\partial t} + \frac{\partial(\rho_L U_L W_S)}{\partial x} + \frac{\partial(\rho_L V_L W_S)}{\partial y} = \frac{\partial}{\partial x} \left(\rho_L D_L^{AB} \frac{\partial W_S}{\partial x} \right) + \frac{\partial}{\partial y} \left(\rho_L D_L^{AB} \frac{\partial W_S}{\partial y} \right) \quad (2.24)$$

In the case that pure water is used as the liquid falling film, the terms including the salt mass fraction (W_S) are neglected in the equations.

2.4.2 Gas Phase

- Gas continuity equation

$$\frac{\partial \rho_M}{\partial t} + \frac{\partial(\rho_M U_M)}{\partial x} + \frac{\partial(\rho_M V_M)}{\partial y} = -\dot{S}_C''' \quad (2.25)$$

- Gas momentum equation in the x direction

$$\frac{\partial(\rho_M U_M)}{\partial t} + \frac{\partial(\rho_M U_M U_M)}{\partial x} + \frac{\partial(\rho_M V_M U_M)}{\partial y} = -\frac{\partial P_M}{\partial x} + \frac{\partial}{\partial x} \left(\mu_M \frac{\partial U_M}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_M \frac{\partial U_M}{\partial y} \right) + \rho_M g_x \quad (2.26)$$

- Gas momentum equation in the y direction

$$\frac{\partial(\rho_M V_M)}{\partial t} + \frac{\partial(\rho_M U_M V_M)}{\partial x} + \frac{\partial(\rho_M V_M V_M)}{\partial y} = -\frac{\partial P_M}{\partial y} + \frac{\partial}{\partial x} \left(\mu_M \frac{\partial V_M}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_M \frac{\partial V_M}{\partial y} \right) + \rho_M g_y \quad (2.27)$$

- Gas energy equation

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_M C_{p,M} T_M) + \frac{\partial}{\partial x} (\rho_M U_M C_{p,M} T_M) + \frac{\partial}{\partial y} (\rho_M V_M C_{p,M} T_M) &= \frac{\partial}{\partial x} \left(k_M \frac{\partial T_M}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_M \frac{\partial T_M}{\partial y} \right) \\ &+ \frac{\partial}{\partial x} \left(\rho_M D_M^{AB} (C_{p,g} - C_{p,v}) \frac{\partial W_a}{\partial x} T_M \right) + \frac{\partial}{\partial y} \left(\rho_M D_M^{AB} (C_{p,g} - C_{p,v}) \frac{\partial W_a}{\partial y} T_M \right) + \dot{S}_T''' \end{aligned} \quad (2.28)$$

- Gas mass fraction equation

$$\frac{\partial(\rho_M W_a)}{\partial t} + \frac{\partial(\rho_M U_M W_a)}{\partial x} + \frac{\partial(\rho_M V_M W_a)}{\partial y} = \frac{\partial}{\partial x} \left(\rho_M D_M^{AB} \frac{\partial W_a}{\partial x} \right) + \frac{\partial}{\partial y} \left(\rho_M D_M^{AB} \frac{\partial W_a}{\partial y} \right) + \dot{S}_W''' \quad (2.29)$$

The pressure, P , in the governing equations is the local relative static pressure. To calculate the flow properties in the liquid and gas phases and the interface, a reference pressure of $P = P_{L,\text{in}}$ is added to the solution relative static pressure. The thermodynamic and transport properties and partial massive enthalpies are calculated based on the local temperature, mass fraction, and pressure using equations in [96]. Source terms $\dot{S}_C'''$, $\dot{S}_T'''$, and $\dot{S}_W'''$ are used to deal with the supersaturation condition when humid air is presented in the system. These terms are thoroughly discussed in Appendix B.

2.4.3 Interface Conditions

At the liquid-gas interface ($y = \delta$) the following conditions are applied to couple the fields in the liquid and gas phases:

- Normal force balance

$$(\hat{n} \cdot \boldsymbol{\tau})_{L,\text{intf}} \cdot \hat{n} + \sigma K = (\hat{n} \cdot \boldsymbol{\tau})_{M,\text{intf}} \cdot \hat{n} \quad (2.30)$$

- Tangential force balance

$$(\hat{n} \cdot \boldsymbol{\tau})_{L,\text{intf}} \cdot \hat{s} - \left. \frac{\partial \sigma}{\partial s} \right|_{L,\text{intf}} = (\hat{n} \cdot \boldsymbol{\tau})_{M,\text{intf}} \cdot \hat{s} \quad (2.31)$$

where $\hat{n}$ and $\boldsymbol{\tau}$ are the local normal unit vector to the interface and the stress tensor, respectively. σ is the surface tension and K is the curvature of the interface. Additionally, $\hat{s}$ is the local tangential unit vector to the interface. In the present work, the surface tension force at the interface has been neglected.

- Continuity of tangential velocity

$$(\vec{V}_t)_{L,\text{intf}} = (\vec{V}_t)_{M,\text{intf}} \quad (2.32)$$

- Continuity of evaporated mass

$$\dot{m}''_{L,\text{intf}} = \dot{m}''_{M,\text{intf}} = \dot{m}''_{\text{evap}} \quad (2.33)$$

- Energy balance

$$k_L \left. \frac{\partial T_L}{\partial y} \right|_{L,\text{intf}} = k_M \left. \frac{\partial T_M}{\partial y} \right|_{M,\text{intf}} - \dot{m}_{\text{intf}}'' h_{fg} \quad (2.34)$$

- Continuity of temperature

$$T_L = T_M = T_{\text{intf}}, \quad T_{\text{intf}} = T(W_{S,\text{intf}}, T_{v,\text{intf}}) \quad (2.35)$$

$T_{v,\text{intf}}$ is equal to the saturation temperature of pure water corresponding to the partial pressure of the vapour at the interface ($P_{v,\text{intf}}^c$), which is calculated using Equation 2.12. Salt-water temperature at the interface is calculated based on the equilibrium salinity and vapour temperature using the correlation presented in Appendix C.

- Impermeability of gas at the interface

$$\rho_M D_M^{AB} \left. \frac{\partial W_a}{\partial y} \right|_{M,\text{intf}} = \dot{m}_{\text{intf}}'' W_{a,\text{intf}} \quad (2.36)$$

- Impermeability of salt at the interface

$$\rho_L D_L^{AB} \left. \frac{\partial W_S}{\partial y} \right|_{L,\text{intf}} = \dot{m}_{\text{intf}}'' W_{S,\text{intf}} \quad (2.37)$$

- Zero pressure gradient in the normal direction at the interface

$$\left(\frac{\partial P_M}{\partial n} \right)_{\text{intf}} = 0 \quad (2.38)$$

2.4.4 Domain and Boundary Condition Definitions

The following boundary conditions, as shown in Figure 2.1 for a vertical channel and in Figure 2.2 for a horizontal tube, are prescribed:

- at the inlet ($x = 0$)

Vertical channel: uniform temperature and mass fraction and fully developed velocity profiles

$$U_L = U_{L,\text{in}}(y), \quad V_L = 0, \quad W_S = W_{S,\text{in}}, \quad T_L = T_{L,\text{in}} \quad \text{for} \quad 0 \leq y \leq \delta_{\text{in}} \quad (2.39)$$

$$U_M = U_{M,\text{in}}(y), \quad V_M = 0, \quad W_a = W_{a,\text{in}}, \quad T_M = T_{M,\text{in}} \quad \text{for} \quad \delta_{\text{in}} \leq y \leq H \quad (2.40)$$

Horizontal Tube: uniform temperature, mass fraction, and velocity

$$U_L = U_{L,\text{in}}, \quad V_{L,\text{in}} = 0, \quad W_S = W_{S,\text{in}}, \quad T_L = T_{L,\text{in}} \quad \text{for} \quad 0 \leq y \leq \delta_{\text{in}} \quad (2.41)$$

$$U_M = U_{M,\text{in}}, \quad V_{M,\text{in}} = 0, \quad W_a = W_{a,\text{in}}, \quad T_M = T_{M,\text{in}} \quad \text{for} \quad \delta_{\text{in}} \leq y \leq H \quad (2.42)$$

- at the boundary beside the liquid phase:

Vertical Channel: constant wall heat flux, no mass transfer, and no slip and no penetration conditions at the wall

$$\frac{\partial T_L}{\partial y} = -\frac{q''_{\text{wall}}}{k_L}, \quad \frac{\partial W_S}{\partial y} = 0, \quad U_L = 0, \quad V_L = 0 \quad (2.43)$$

Horizontal tube: constant temperature, no mass transfer, and no slip and no penetration conditions at the tube wall

$$T_L = T_{\text{wall}}, \quad \frac{\partial W_S}{\partial n} = 0, \quad U_L = 0, \quad V_L = 0 \quad (2.44)$$

Zero temperature gradient, no mass transfer, zero U velocity gradient, and no penetration conditions at symmetry lines L_1 and L_2

$$\frac{\partial T_L}{\partial y} = 0, \quad \frac{\partial W_S}{\partial y} = 0, \quad \frac{\partial U_L}{\partial y} = 0, \quad V_L = 0 \quad (2.45)$$

- at the boundary beside the gas phase ($y = H$):

zero temperature and U velocity gradients and no penetration condition for the gas

$$\frac{\partial T_M}{\partial y} = 0, \quad \frac{\partial W_a}{\partial y} = 0, \quad \frac{\partial U_M}{\partial y} = 0, \quad V_M = 0 \quad (2.46)$$

- at the outlet ($x = L$)

fully developed conditions in both phases

$$\begin{aligned} \frac{\partial T_L}{\partial x} = 0, \quad \frac{\partial W_S}{\partial x} = 0, \quad \frac{\partial U_L}{\partial x} = 0, \quad \frac{\partial V_L}{\partial x} = 0 \quad \text{for} \quad 0 \leq y \leq \delta \quad (2.47) \\ \frac{\partial T_M}{\partial x} = 0 \quad \text{or} \quad T_M = T_{\text{intf}} \quad (\text{if} \quad U_M < 0), \quad \frac{\partial W_a}{\partial x} = 0 \quad \text{or} \quad W_a = W_{a,\text{intf}} \quad (\text{if} \quad U_M < 0), \\ \frac{\partial U_M}{\partial x} = 0, \quad \frac{\partial V_M}{\partial x} = 0 \quad \text{for} \quad \delta \leq y \leq H \quad (2.48) \end{aligned}$$

In the elliptic model, the relative pressure at the outlet is specified as a reference pressure and the inlet pressure is determined from the solution.

Once the geometry, the properties, and the interface and boundary conditions are prescribed, the elliptic model is used to determine the U and V velocities, pressure, and temperature in both phases and the salt mass fraction and air mass fraction in the liquid and gas phases, respectively. The location of the phase interface is determined by an adaptive-grid Eulerian method that is described in the following section.

2.4.5 Interface Moving Strategy

The evaporation phenomenon is a problem involving a moving boundary, where the position of the interface between the two phases needs to be included in the detailed solution. A major contribution of this work is the advancement of an accurate phase interface tracking scheme.

After obtaining the solution field on a fixed grid, the interface location is determined by applying an integral liquid mass balance (ILMB) to each axial column of liquid at the end of each time step using the following method:

$$\int_0^{\delta_i} \rho_{L,e} U_{L,e} dy = \int_0^{\delta_{i-1}} \rho_{L,w} U_{L,w} dy + \dot{m}'_{\text{intf}} \quad (2.49)$$

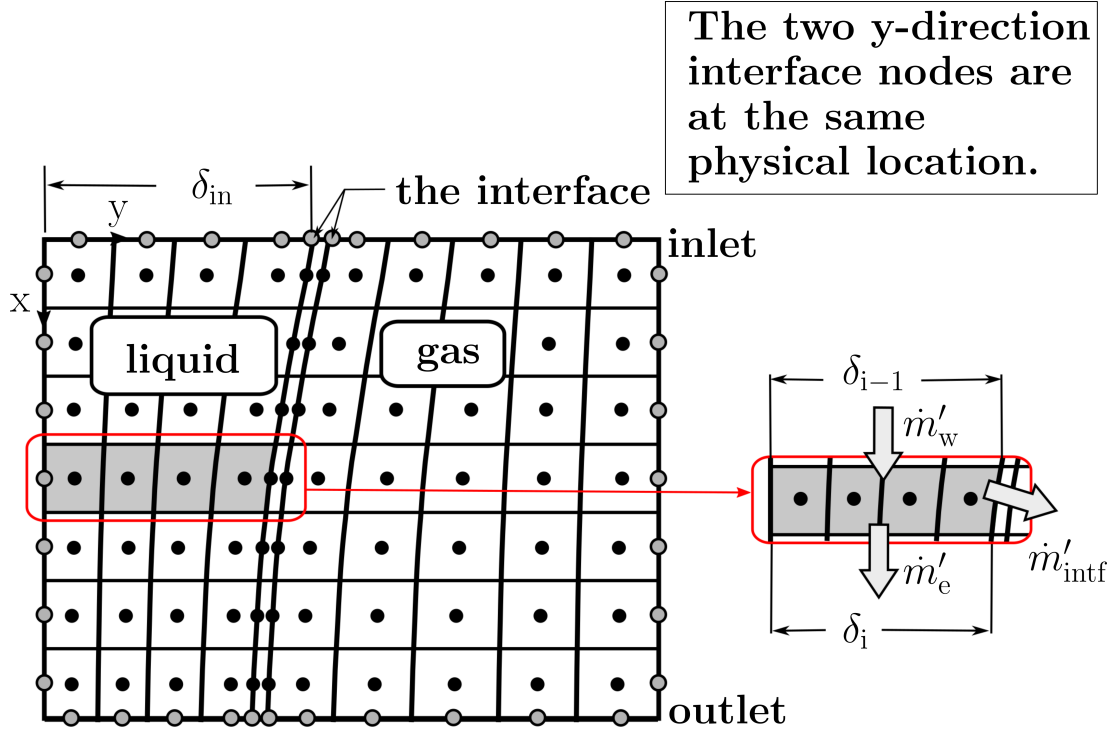


Figure 2.3: Grid information of the phases and a typical liquid region used in ILMB method; the interface nodes are shown separated for illustration purposes.

This equation is defined for a vertical channel grid, with the east and west faces of the control volumes being normal to the x axis. The ILMB equation is provided in a general form in Section 4.3.5. In Equation (2.49), δ_{i-1} and δ_i represent the film thicknesses at the axial positions of the west and east faces, respectively, of a typical control volume column in the liquid. The mass balance is illustrated schematically in Figure 2.3. Equation (2.49) indicates that the difference between the total mass flow rate through the west faces of the control volumes and the total mass flow rate exiting the column through the east faces must equal the evaporated mass flow rate crossing the interface. Starting from the inlet of the domain, the downstream side film thickness, δ_i , is obtained using the upstream side film thickness, δ_{i-1} , and the evaporated mass at the interface, $\dot{m}'_{intf}$, by applying a forward marching scheme. The details of the grid are described later in Chapter 3 and further details about discretised form of the ILMB equation are presented in Section 4.3.5.

Chapter 3

Discretisation of the Domain

3.1 Parabolic Model

3.1.1 Introduction

In order to maintain a structured grid system as the film thickness varies along the x direction, a coordinate transformation is applied in the parabolic model. In this setup, an index in the x direction represents a station, each of which includes a column of control volumes. At the first station, a set of parabolic governing equations is solved based on the inlet conditions shown in Figure 2.1. The finite volume method is used for discretization in this numerical approach. With the inlet conditions known, the solution progresses sequentially from one station to the next along the channel. This approach is referred to as a marching scheme. The details of the coordinate transformation will be explained in the following sections.

3.1.2 Coordinate Transformation

The Cartesian coordinates x and y are transformed into χ and η following the work by Siow [95]:

$$\chi = x \quad \text{for } x \geq 0, \quad (3.1)$$

$$\eta = \frac{y}{\delta} \quad \text{for } 0 \leq y \leq \delta, \quad (3.2)$$

$$\eta = \frac{y - \delta}{H - \delta} + 1 \quad \text{for } \delta \leq y \leq H. \quad (3.3)$$

This transformation enables the grid boundary to adjust to variations in δ along the channel while preserving a structured grid in both phases. In the new coordinate system, the liquid region is clearly defined as $0 \leq \eta \leq 1$, and the gas region is defined as $1 \leq \eta \leq 2$. Despite the decrease of

film thickness in the x direction, the interface consistently remains at $\eta = 1$. Consequently, all governing equations and boundary conditions for both phases need to be rewritten according to the new coordinates. In the following section only the final versions of the transformed equations are presented. Details of the derivations can be found in Appendix B of Siow [95].

3.1.3 Transformed Governing Equations

The liquid phase governing equations, Equations (2.1) to (2.3), become:

$$\frac{\partial(\delta\rho_L U_L)}{\partial\chi} + \frac{\partial(J_L'')}{\partial\eta} = 0 \quad (3.4)$$

$$\frac{\partial(\delta\rho_L U_L U_L)}{\partial\chi} + \frac{\partial(J_L'' U_L)}{\partial\eta} = -\delta \frac{dP}{d\chi} + \frac{\partial}{\partial\eta} \left(\frac{\mu_L}{\delta} \frac{\partial U_L}{\partial\eta} \right) + \delta\rho_L g_x \quad (3.5)$$

$$\frac{\partial}{\partial\chi} (\delta\rho_L U_L C_{p,L} T_L) + \frac{\partial}{\partial\eta} (J_L'' C_{p,L} T_L) = \frac{\partial}{\partial\eta} \left(\frac{k_L}{\delta} \frac{\partial T_L}{\partial\eta} \right) \quad (3.6)$$

The gas phase governing equations, Equations (2.4) to (2.7), become:

$$\frac{\partial((H-\delta)\rho_M U_M)}{\partial\chi} + \frac{\partial(J_M'')}{\partial\eta} = 0 \quad (3.7)$$

$$\frac{\partial((H-\delta)\rho_M U_M U_M)}{\partial\chi} + \frac{\partial(J_M'' U_M)}{\partial\eta} = -(H-\delta) \frac{dP}{d\chi} + \frac{\partial}{\partial\eta} \left(\frac{\mu_M}{(H-\delta)} \frac{\partial U_M}{\partial\eta} \right) + (H-\delta)\rho_M g_x \quad (3.8)$$

$$\begin{aligned} \frac{\partial}{\partial\chi} ((H-\delta)\rho_M U_M C_{p,M} T_M) + \frac{\partial}{\partial\eta} (J_M'' C_{p,M} T_M) = \\ \frac{\partial}{\partial\eta} \left(\frac{k_M}{H-\delta} \frac{\partial T_M}{\partial\eta} \right) + \frac{\partial}{\partial\eta} \left(\frac{\rho_M D_M^{AB}}{H-\delta} \frac{\partial W_a}{\partial\eta} (C_{p,g} - C_{p,v}) T_M \right) \end{aligned} \quad (3.9)$$

$$\frac{\partial[(H-\delta)(\delta\rho_M U_M W_a)]}{\partial\chi} + \frac{\partial(J_M'' W_a)}{\partial\eta} = \frac{\partial}{\partial\eta} \left(\frac{\rho_M D_M^{AB}}{H-\delta} \frac{\partial W_a}{\partial\eta} \right) \quad (3.10)$$

The continuity of velocity and shear, Equation (2.9), and mass, Equation (2.10), at the interface become:

$$U_L = U_M, \quad \frac{\mu_L}{\delta} \frac{\partial U_L}{\partial \eta} = \frac{\mu_M}{(H-\delta)} \frac{\partial U_M}{\partial \eta} \quad (3.11)$$

$$J''_{L,\text{intf}} = J''_{M,\text{intf}} \quad (3.12)$$

The impermeability of air, Equation (2.13), and continuity of energy, Equation (2.14), at the interface become:

$$-\frac{\rho_M D^{AB}}{\delta} \frac{\partial W_a}{\partial \eta} = J''_{\text{intf}} W_a \quad (3.13)$$

$$\frac{k_L}{\delta} \frac{\partial T_L}{\partial \eta} = \frac{k_M}{(H-\delta)} \frac{\partial T_M}{\partial \eta} - J''_{\text{intf}} h_{fg} \quad (3.14)$$

Overall mass balance, Equation (2.8), becomes:

$$\int_0^1 \delta \rho_L U_L d\eta + \int_1^2 (H-\delta) \rho_M U_M d\eta = \dot{m}'_{L,\text{in}} + \dot{m}'_{M,\text{in}} \quad (3.15)$$

The transformed governing equations are solved for U_L , J''_L , T_L , U_M , J''_M , T_M , and W_a and scalar unknowns δ and $dP/d\chi$ using a marching scheme. In the formulation of the solution variables, the transverse velocity, V , is replaced by J'' , where:

$$J''_L = \rho_L V_L + \rho_L U_L \eta \frac{d\delta}{d\chi} \quad (3.16)$$

$$J''_M = \rho_M V_M + \rho_M U_M (\eta - 2) \frac{d\delta}{d\chi} \quad (3.17)$$

J'' is the mass flux in the η direction (e.g., $J''_{\text{intf}} = \dot{m}''_{\text{intf}}$).

3.1.4 Grid system

The coordinate transformation facilitates dividing the liquid and gas regions to two equal logically rectangular domains. The Figure 3.1 illustrates a simplified grid, with $N_x \times N_{y,L}$ control volumes

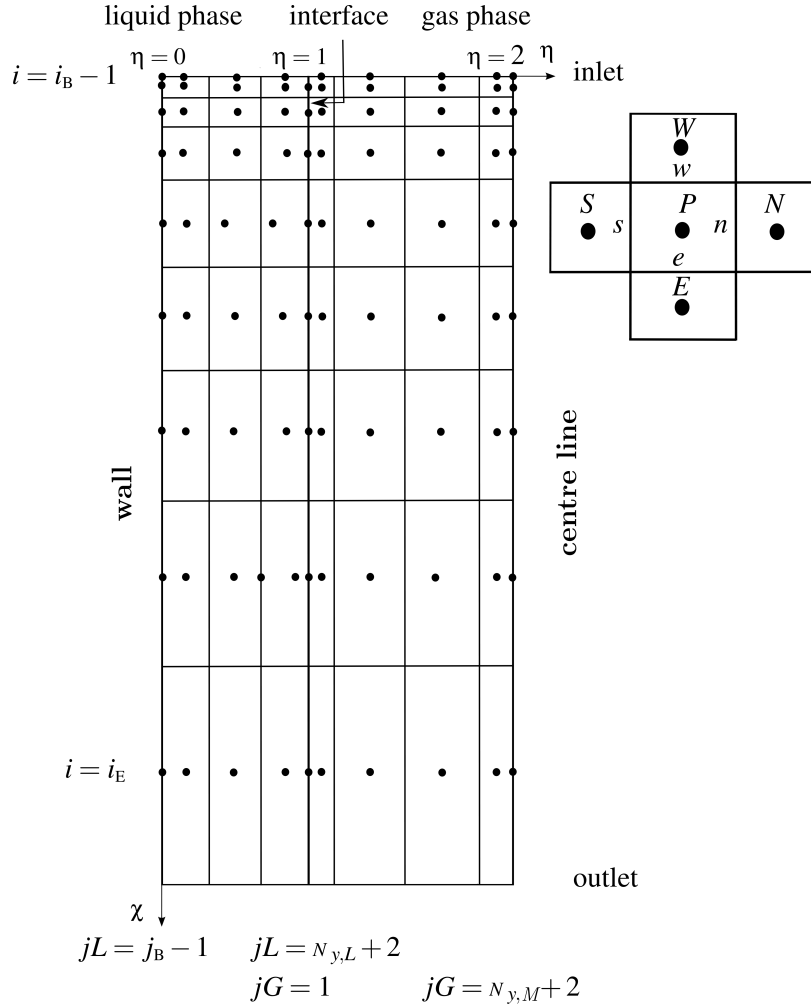


Figure 3.1: Grid nomenclature in transformed coordinates.

in the liquid region and $N_x \times N_{y,M}$ control volumes in the gas region. The same number of control volumes is used in the χ direction for both phases. Each rectangle in the grid represents a control volume with a central node where indexing is applied. The index i denotes the station number in the χ direction, jL labels the nodes in the η direction for the liquid region (starting from the wall), and jG labels the nodes in the η direction for the gas region (starting from the interface).

The grid spacings in the χ direction are uniform and very fine at the beginning of the channel to capture the sharp gradients at the entrance. The grid then expands exponentially and becomes coarser at the end of the channel. In the η direction the grid spacing is different in the liquid and the

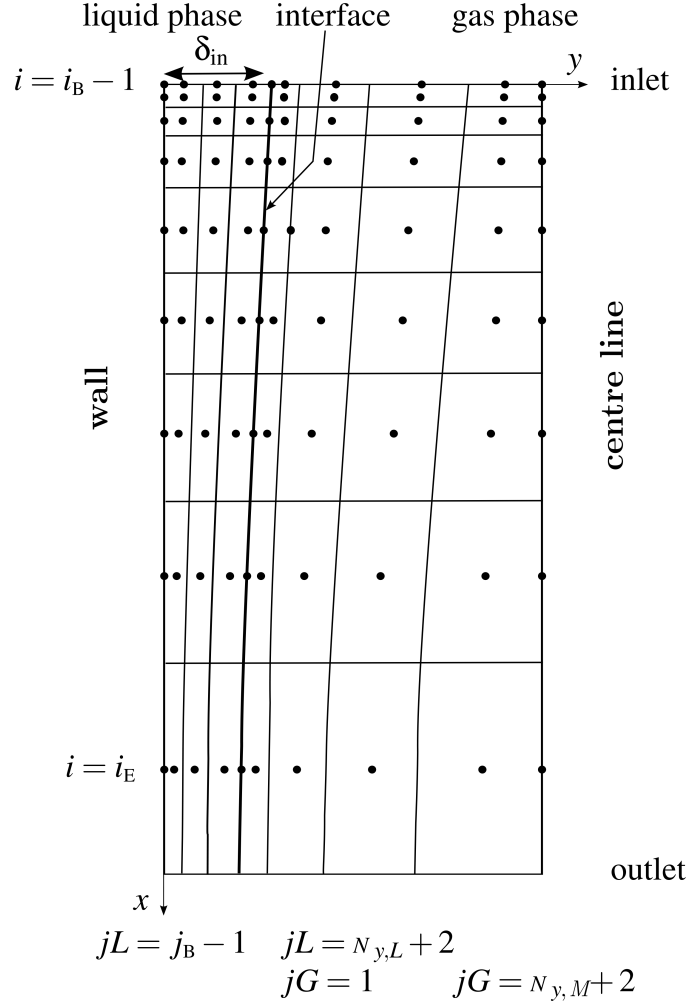


Figure 3.2: Grid nomenclature in Cartesian coordinates.

gas regions. A sufficient number of nodes is used in the solution film in order to capture the changes in temperature and mass fraction of the film at the interface. The gas phase also has a fine grid adjacent to the interface to ensure implementing the continuity of the shear at the interface. Control volumes at the inlet ($i = i_B - 1$), control volumes at the liquid–gas interface ($jL = N_{y,L} + 2$, $jG = 1$), and control volumes located at the lower and upper boundaries ($jL = j_B - 1$ and $jG = N_{y,M} + 2$) all have zero thickness. Field variables such as U , T , and W_a are stored at the nodal point, whereas J is stored at the north face of a control volume (the mass flow rate is stored instead of the mass flux value, J''). J is always normal to the north face of the control volume. Because the film thickness δ

and pressure gradient $\frac{dP}{d\chi}$ are constant at a given χ location, they have a single value at each station.

Figure 3.2 represents the actual domain in the $x-y$ coordinate system, showing the film thickness starting at $x = 0$ and decreasing along the channel.

3.2 Elliptic Model

3.2.1 Introduction

A non-orthogonal structured mesh is used to discretise the solution domain in the elliptic model. The use of transfinite interpolation in mesh generation as described in Wang et al. [97] provides the capability of dividing the domain to more than one panel in each coordinate direction. In each panel, nodes are distributed independently to control mesh refinement in desired areas (e.g., near a wall or interface). In this work, separate panels are used for the liquid and gas regions. These two regions are separated by a smooth interface. The non-orthogonal mesh enables the precise grid adaption to the interface changing shape along a channel or over a tube. The gas region bottom boundary is spatially coincident with the liquid region top boundary. The liquid-gas interface consists of two rows of zero-width control volumes as shown in Figure 3.3. Each row represents the interface of one of the phases. Figure 3.3 shows a sample complete computational grid for liquid-gas flow in a channel. In the y direction, the liquid region has $N_{y,L}$ uniform control volumes in one panel and the gas region has total number of $N_{y,M}$ control volumes that could be divided into more than one panel if necessary. In the x direction, N_x interior control volumes are used.

As shown in Figure 3.3, j_{BL} to $j_{EL} + 1$ and $j_{BG} - 1$ to $j_{EG} + 1$ belong to the liquid region and gas region, respectively. Each control volume is identified by a pair of indices (i, j) that is changing in an organized fashion. The i index proceeds from $i_B = 2$ for the first interior control volume on the west side of the domain to $i_E = N_x + 1$ for the last interior control volume on the east. Along the y direction, the j index proceeds from $j_B = 2$ to $j_{EL} + 1 = N_{y,L} + 2$ in the liquid region and from $j_{BG} - 1 = N_{y,L} + 3$ to $j_{EG} = N_{y,L} + N_{y,M} + 3$ in the gas region.

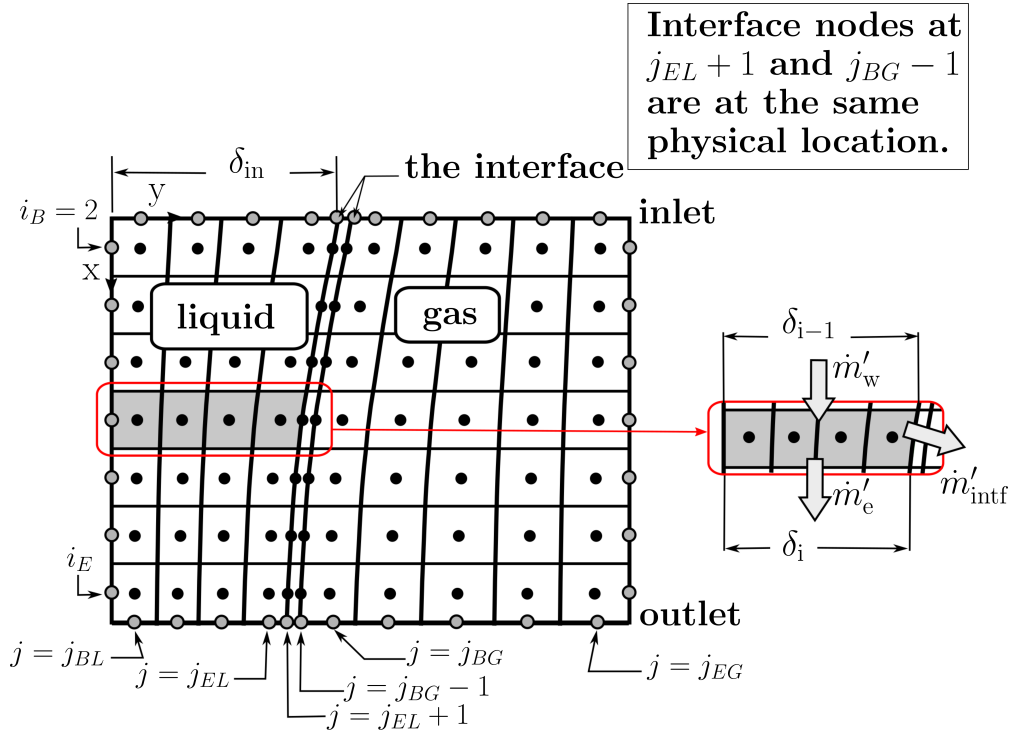


Figure 3.3: Grid information in the liquid and gas regions; the spacing between the nodes at the interface is exaggerated for illustration purposes.

The zero-width control volumes of the interface are located at $j = j_{EL} + 1$ and $j = j_{BG} - 1$ which are at the same physical location. In Figure 3.3, however, the spacing between these two rows are exaggerated to emphasize that they are two separate sets of nodes. The domain boundary nodes are also zero-width control volumes that are used to implement the boundary conditions and specified by a grey colour in the figure.

3.2.2 Grid Nomenclature

A typical control volume P and its eight neighbours are presented in Figure 3.4. The neighbouring control volumes are referred by compass notation relative to the centre node P . The faces of the central control volume, P , are distinguished by lower case letters according to their relative location

to the centre. Each control volume consists of four quadrants as shown in Figure 3.5. These

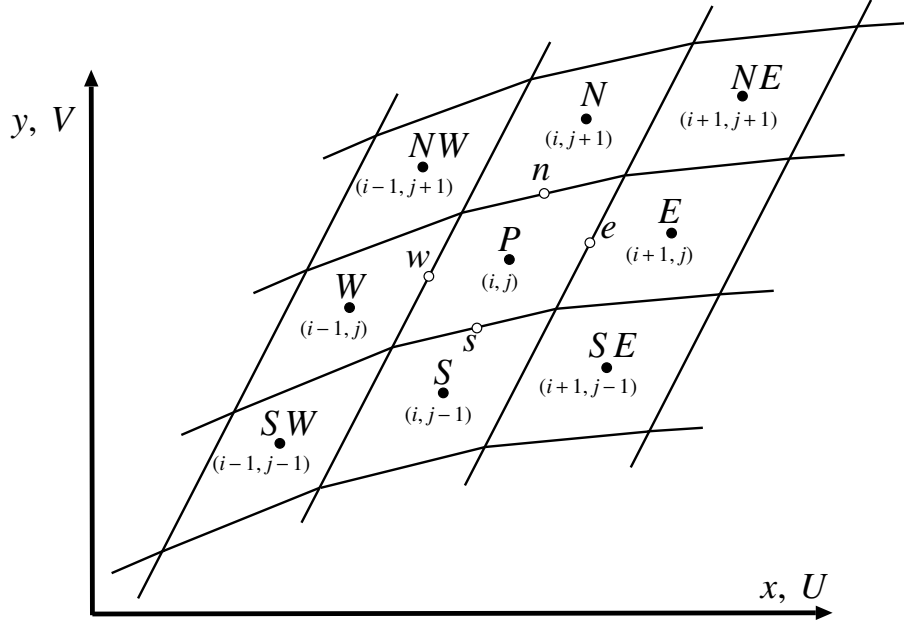


Figure 3.4: Computational molecule: indexing and notation.

quadrants are referred to by geographical directions, northeast (NE), southeast (SE), northwest (NW), and southwest (SW). The points on the faces of the control volume P are located at the centre of each face. The location of centre node P is indicated by $(X_{SW}(i, j), Y_{SW}(i, j))$. The coordinates of points P, e, n, and ne (the solid points in Figure 3.5) are calculated and stored for each control volume. The location of other points are derived from the locations stored for neighbouring control volumes.

The nomenclature for control volume distances, areas, and volumes is shown in Figure 3.6. The distances are calculated based on the coordinates of the first and second endpoints. Each quadrant in a control volume is divided into two triangles. The areas of these two triangles are calculated and then added to calculate the area of each quadrant. Unit depth is used to compute the areas and volumes.

The accurate evaluation of different quantities in non-orthogonal grid needs introduction of some local directional unit vectors, because the non-orthogonal grid will not be necessarily aligned

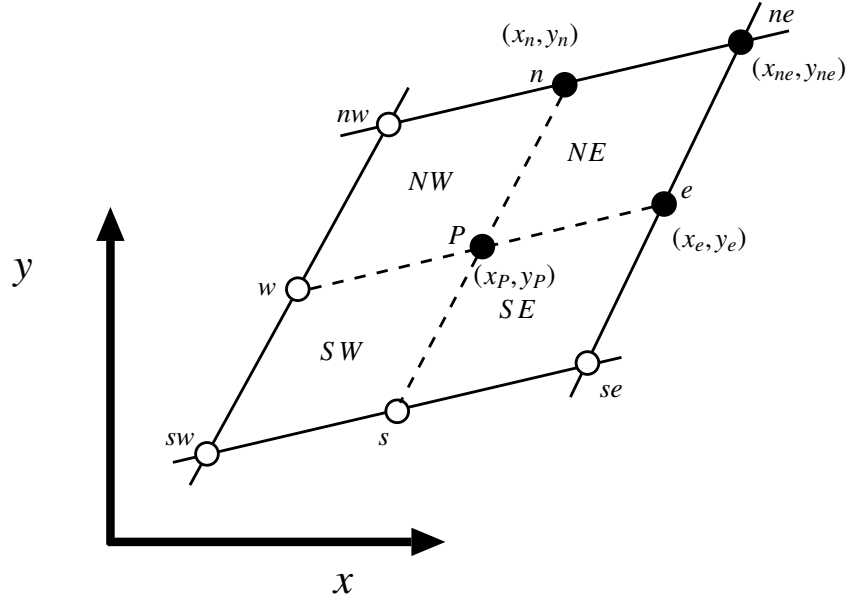


Figure 3.5: Coordinates of control volume points and quadrant notation.

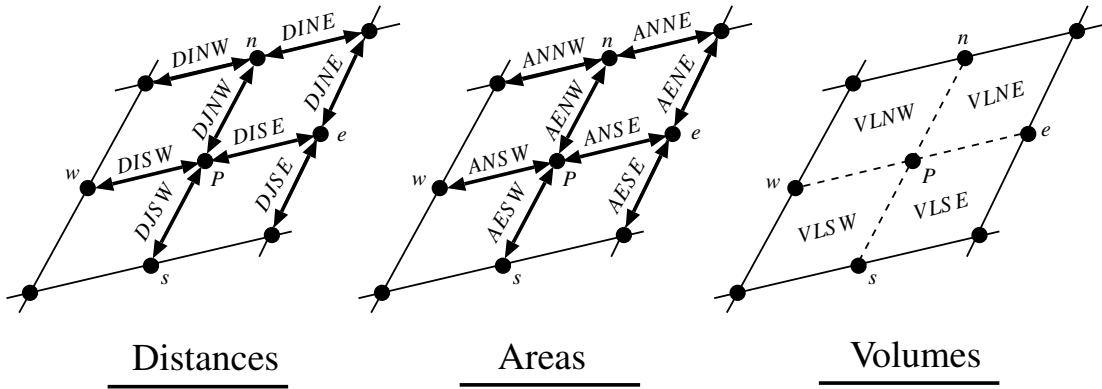


Figure 3.6: Distances, areas and volumes of a control volume.

with the Cartesian coordinate directions. Figure 3.7 shows directions of unit vectors at the east and north faces and the central node of the main control volume. In general, the $\hat{s}$ vectors denote moving along the i index and the $\hat{t}$ vectors denote moving along the j index and they are not necessarily aligned with the Cartesian unit vectors $\hat{i}$ and $\hat{j}$. The unit vector $\hat{n}$ is normal to the faces of the P control volume. The unit vectors on the east face, north face, and centre of the control

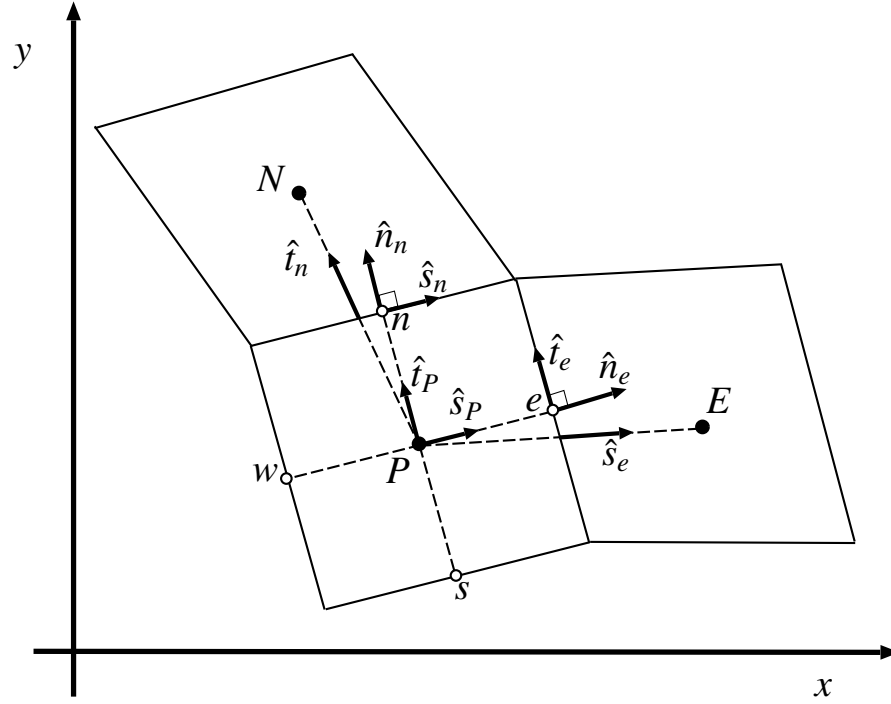


Figure 3.7: Grid directional unit vectors.

volume are referred by subscripts e , n , and P , respectively. The unit vectors $\hat{t}_e$ and $\hat{s}_n$ are tangent to the east and north face, respectively. $\hat{s}_e$ gives the direction of the line that connects nodal point P and its first neighbouring node on the east. $\hat{t}_n$ gives the direction of the line that connects nodal point P and its first neighbouring node on the north. $\hat{t}_P$ and $\hat{s}_P$ determine the directions of the imaginary lines between the nodal point P and the central points of its faces. The unit vectors at the west and south faces of the control volume P , (i, j) , are identical to those at east and north of the control volumes $(i - 1, j)$ and $(i, j - 1)$, respectively. The unit vectors shown in Figure 3.7 are defined in terms of their component in the x and y directions as following:

$$\left. \begin{aligned} \hat{n}_n &= \frac{\partial x}{\partial n} \Big|_n \hat{i} + \frac{\partial y}{\partial n} \Big|_n \hat{j} = n_{xn} \hat{i} + n_{yn} \hat{j} \\ \hat{n}_e &= \frac{\partial x}{\partial n} \Big|_e \hat{i} + \frac{\partial y}{\partial n} \Big|_e \hat{j} = n_{xe} \hat{i} + n_{ye} \hat{j} \\ \hat{s}_n &= \frac{\partial x}{\partial s} \Big|_n \hat{i} + \frac{\partial y}{\partial s} \Big|_n \hat{j} = s_{xn} \hat{i} + s_{yn} \hat{j} \\ \hat{s}_e &= \frac{\partial x}{\partial s} \Big|_e \hat{i} + \frac{\partial y}{\partial s} \Big|_e \hat{j} = s_{xe} \hat{i} + s_{ye} \hat{j} \\ \hat{s}_p &= \frac{\partial x}{\partial s} \Big|_p \hat{i} + \frac{\partial y}{\partial s} \Big|_p \hat{j} = s_{xp} \hat{i} + s_{yp} \hat{j} \\ \hat{t}_n &= \frac{\partial x}{\partial t} \Big|_n \hat{i} + \frac{\partial y}{\partial t} \Big|_n \hat{j} = t_{xn} \hat{i} + t_{yn} \hat{j} \\ \hat{t}_e &= \frac{\partial x}{\partial t} \Big|_e \hat{i} + \frac{\partial y}{\partial t} \Big|_e \hat{j} = t_{xe} \hat{i} + t_{ye} \hat{j} \\ \hat{t}_p &= \frac{\partial x}{\partial t} \Big|_p \hat{i} + \frac{\partial y}{\partial t} \Big|_p \hat{j} = t_{xp} \hat{i} + t_{yp} \hat{j} \end{aligned} \right\} \quad (3.18)$$

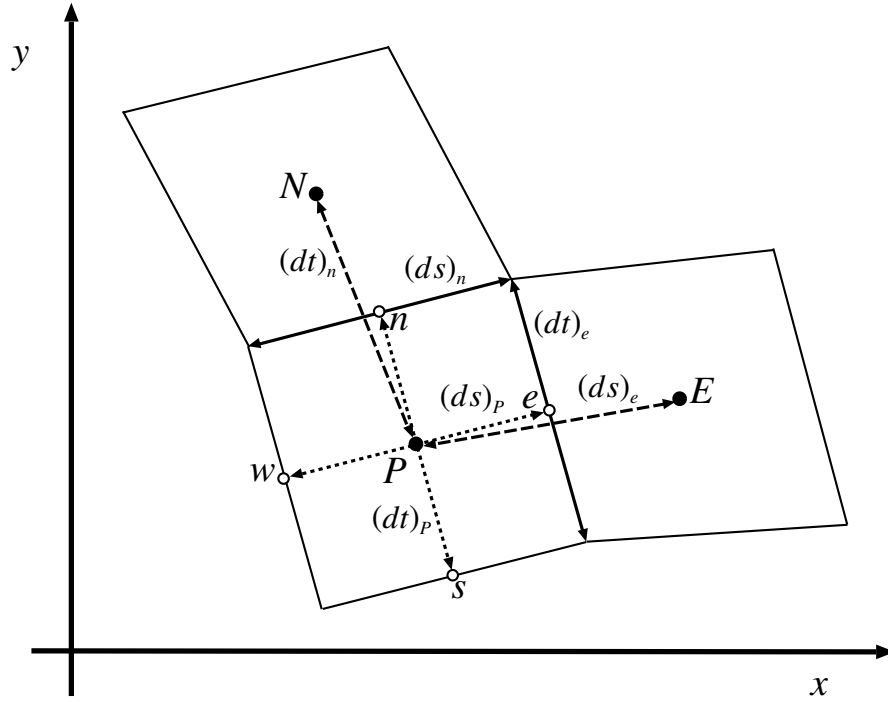


Figure 3.8: Location of distance variables.

The variables assigned to distances used in the computations for a non-orthogonal grid are shown in Figure 3.8. These distances could be calculated using the definitions presented in Figure 3.6. For nodal point P, $(ds)_P$ and $(dt)_P$ are:

$$(ds)_{P_{(i,j)}} = DISW_{(i,j)} + DISE_{(i,j)} \quad (3.19)$$

$$(dt)_{P_{(i,j)}} = DJSW_{(i,j)} + DJNW_{(i,j)} \quad (3.20)$$

The distances $(dt)_e$ and $(ds)_n$ along the east and north faces are defined as:

$$(dt)_{e_{(i,j)}} = DJSE_{(i,j)} + DJNE_{(i,j)} \quad (3.21)$$

$$(ds)_{n_{(i,j)}} = DINW_{(i,j)} + DINE_{(i,j)} \quad (3.22)$$

Equations (3.23) and (3.24) calculate the distance between node P and node E along the $\hat{s}_e$ vector and the distance between node P and node N along the $\hat{t}_n$ vector:

$$(ds)_{e_{(i,j)}} = \sqrt{\left(XSW_{(i+1,j)} - XSW_{(i,j)}\right)^2 + \left(YSW_{(i+1,j)} - YSW_{(i,j)}\right)^2} \quad (3.23)$$

$$(dt)_{n_{(i,j)}} = \sqrt{\left(XSW_{(i,j+1)} - XSW_{(i,j)}\right)^2 + \left(YSW_{(i,j+1)} - YSW_{(i,j)}\right)^2} \quad (3.24)$$

Using the definitions for distances in a non-orthogonal grid, the components of the unit vectors

are defined as follows:

$$\left. \begin{aligned} \hat{n}_{n(i,j)} &= \frac{-(YNE_{(i,j)} - YNE_{(i-1,j)})}{(ds)_{n(i,j)}} \hat{i} + \frac{(XNE_{(i,j)} - XNE_{(i-1,j)})}{(ds)_{n(i,j)}} \hat{j} \\ \hat{n}_{e(i,j)} &= \frac{(YNE_{(i,j)} - YNE_{(i,j-1)})}{(dt)_{e(i,j)}} \hat{i} + \frac{-(XNE_{(i,j)} - XNE_{(i,j-1)})}{(dt)_{e(i,j)}} \hat{j} \\ \hat{s}_{n(i,j)} &= \frac{(XNE_{(i,j)} - XNE_{(i-1,j)})}{(ds)_{n(i,j)}} \hat{i} + \frac{(YNE_{(i,j)} - YNE_{(i-1,j)})}{(ds)_{n(i,j)}} \hat{j} \\ \hat{s}_{e(i,j)} &= \frac{(XSW_{(i+1,j)} - XSW_{(i,j)})}{(ds)_{e(i,j)}} \hat{i} + \frac{(YSW_{(i+1,j)} - YSW_{(i,j)})}{(ds)_{e(i,j)}} \hat{j} \\ \hat{s}_{p(i,j)} &= \frac{(XSE_{(i,j)} - XSE_{(i-1,j)})}{(ds)_{p(i,j)}} \hat{i} + \frac{(YSE_{(i,j)} - YSE_{(i-1,j)})}{(ds)_{p(i,j)}} \hat{j} \\ \hat{t}_{n(i,j)} &= \frac{(XSW_{(i,j+1)} - XSW_{(i,j)})}{(dt)_{n(i,j)}} \hat{i} + \frac{(YSW_{(i,j+1)} - YSW_{(i,j)})}{(dt)_{n(i,j)}} \hat{j} \\ \hat{t}_{e(i,j)} &= \frac{(XNE_{(i,j)} - XNE_{(i,j-1)})}{(dt)_{e(i,j)}} \hat{i} + \frac{(YNE_{(i,j)} - YNE_{(i,j-1)})}{(dt)_{e(i,j)}} \hat{j} \\ \hat{t}_{p(i,j)} &= \frac{(XNW_{(i,j)} - XNW_{(i,j-1)})}{(dt)_{p(i,j)}} \hat{i} + \frac{(YNW_{(i,j)} - YNW_{(i,j-1)})}{(dt)_{p(i,j)}} \hat{j} \end{aligned} \right\} \quad (3.25)$$

3.2.3 Grid Expansion Factor

To refine the grid in the desired regions where rapid changes in solution field variables occur, an expansion factor could be applied to the boundaries of each panel in the grid domain. An expansion factor is defined such that the ratio of the length of the neighbouring control volume edges along a grid boundary is fixed. This geometric expansion factor can be used independently at each side of a grid segment. Equation (3.26) shows the expansion factor along the south boundary of a grid:

$$S = \frac{(ds)_{i+1,j_B-1}}{(ds)_{i,j_B-1}} \quad (3.26)$$

The grid cells are expanding if $S > 1$, contracting if $S < 1$, and uniform if $S = 1$. When the control volumes are non-uniformly spaced between the vertices of the grid in one panel, it is crucial to ensure smooth transition between grid panels.

3.2.4 Grid Assembly

Applying a panelling technique provides the advantage of producing grids that matches the shape of a complicated solution domain and controlling mesh refinement where it is required. In the case of a parallel plate channel, two separate panels are used for the liquid and the gas regions. In the y direction, the liquid region has $N_{y,L}$ uniform control volumes, and the gas region has $N_{y,M}$ control volumes in one panel. In the gas region, the mesh is refined adjacent to the interface. In the x direction only one panel with an expanding grid is used in each phase. There is a total of two panels in the configuration.

In the case of a horizontal tube, more panels and some with an arc along their edges are required. Figure 3.9 shows an illustrative example of grid assembly around a tube. In this example, twenty-one panels are used to construct the overall computational domain. In the y direction, one panel in the liquid region (NY1) and two panels in the gas region are used (NY2 and NY3). In the x direction, the liquid and gas regions are divided to seven panels, e.g. panels NX1 and NX2 cover the falling film before the tube top stagnation point, panels NX3, NX4, and NX5 cover the film around the tube, and panels NX6 and NX7 cover the liquid film after the bottom stagnation point. The control volumes are uniformly spaced in the y direction in the liquid and are refined in the gas region toward the interface. To resolve the flow near the top and bottom of the tube accurately, a sufficient number of nodes are required in the panels 2, 3, 5, and 6.

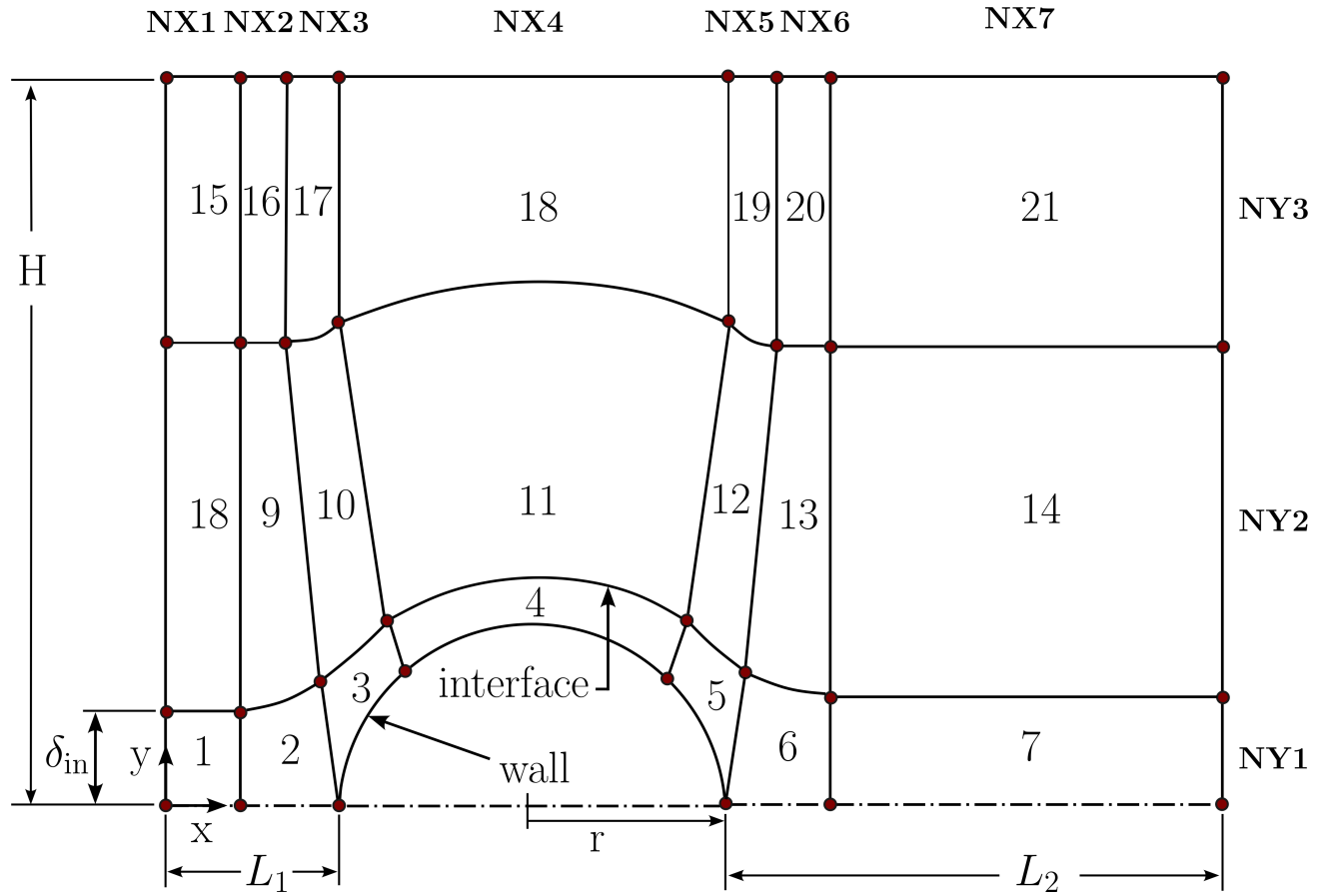


Figure 3.9: Example of grid assembly for falling film evaporation over a horizontal tube.

Chapter 4

Numerical Solution Method

4.1 Introduction

In this chapter, the partial differential equations in the liquid and gas phases are discretised using a finite volume method [98] to obtain a set of algebraic equations for solution variables. The details of the discretisation approaches in the parabolic and elliptic models are presented in the following sections.

4.2 Discretisation of the Parabolic Model Governing Equations

The transformed governing equations are integrated over a typical interior control volume of thickness $d\eta$ and length $d\chi$ using a finite volume method. The resulting algebraic equations require north, south, east, and west face values for all the variables and properties. Plus variable gradients are needed at north and south faces of a control volume. All the properties and the field variables are stored at the centre of a control volume. In addition, a Newton-Raphson Linearisation is used for all the non-linear terms. The details of the methods followed in discretising the governing equations will be discussed in the following sections.

4.2.1 Face values for Variables

The east and west values for $\Phi = \{U_L, T_L, U_M, T_M, W_a\}$, is calculated using the upwind scheme:

$$\Phi_e = \Phi_P, \quad \Phi_w = \Phi_W \quad (4.1)$$

At the north and south faces, an exponential differencing scheme (EDS) is applied:

$$\Phi_n = (0.5 + \alpha_n) \Phi_P + (0.5 - \alpha_n) \Phi_N, \quad \Phi_s = (0.5 + \alpha_s) \Phi_S + (0.5 - \alpha_s) \Phi_P \quad (4.2)$$

The exponential differencing scheme is also used to determine the derivatives at the north and south faces:

$$\left. \frac{\partial \Phi}{\partial \eta} \right|_n = \beta_n \frac{\Phi_N - \Phi_P}{\eta_N - \eta_P}, \quad \left. \frac{\partial \Phi}{\partial \eta} \right|_s = \beta_s \frac{\Phi_P - \Phi_S}{\eta_P - \eta_S} \quad (4.3)$$

where,

$$\alpha_n = \frac{0.5 \text{Pe}_n^2}{5 + \text{Pe}_n^2}, \quad \alpha_s = \frac{0.5 \text{Pe}_s^2}{5 + \text{Pe}_s^2} \quad (4.4)$$

$$\beta_n = \frac{1 + 0.005 \text{Pe}_n^2}{1 + 0.05 \text{Pe}_n^2}, \quad \beta_s = \frac{1 + 0.005 \text{Pe}_s^2}{1 + 0.05 \text{Pe}_s^2} \quad (4.5)$$

For the liquid region ($0 \leq \eta \leq 1$):

$$\text{Pe}_n = \frac{\delta J_n'' (\eta_N - \eta_P)}{D_n}, \quad \text{Pe}_s = \frac{\delta J_s'' (\eta_P - \eta_S)}{D_s} \quad (4.6)$$

For the gas region ($1 \leq \eta \leq 2$):

$$\text{Pe}_n = \frac{(H - \delta) J_n'' (\eta_N - \eta_P)}{D_n}, \quad \text{Pe}_s = \frac{(H - \delta) J_s'' (\eta_P - \eta_S)}{D_s} \quad (4.7)$$

The diffusion coefficient D for U , T , and W_a equations is μ , $\frac{k}{C_p}$, and ρD^{AB} , respectively. The normal mass flow rate, J , is stored at the north face of each control volume:

$$J_n = J_P, \quad J_s = J_S \quad (4.8)$$

The film thickness is assumed to vary linearly across a station:

$$\delta_e = 2\delta_P - \delta_W \quad (4.9)$$

4.2.2 Face Values for Properties

The east and west face values for the thermodynamic properties (ρ, μ, k, C_p , and D^{AB}) are determined using the upwind scheme. For example, the value of density at the east and west faces are calculated as:

$$\rho_e = \rho_P, \quad \rho_w = \rho_W \quad (4.10)$$

The north and south face values are evaluated using a harmonic mean:

$$\rho_n = \frac{\rho_P \rho_N}{\mathcal{W}_n \rho_P + (1 - \mathcal{W}_n) \rho_N}, \quad \rho_s = \frac{\rho_S \rho_P}{\mathcal{W}_s \rho_S + (1 - \mathcal{W}_s) \rho_P} \quad (4.11)$$

where,

$$\mathcal{W}_n = \frac{\eta_N - \eta_n}{\eta_N - \eta_P}, \quad \mathcal{W}_s = \frac{\eta_P - \eta_s}{\eta_P - \eta_S} \quad (4.12)$$

4.2.3 Newton-Raphson Linearisation

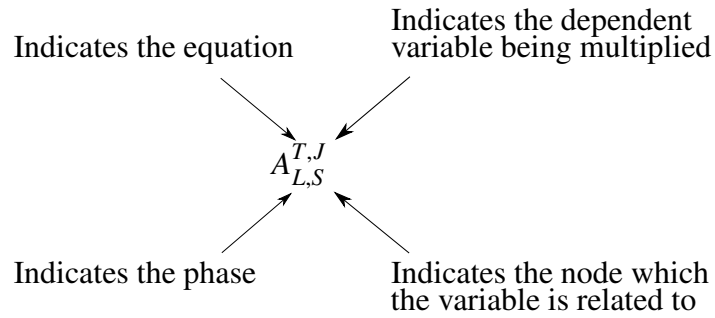
If $\Psi = f(\Phi_1, \Phi_2, \Phi_3)$ and Φ_1, Φ_2 , and Φ_3 are one of the field variables $\{U_L, T_L, J_L, U_M, T_M, J_M, W_a, \delta, \frac{dP}{d\chi}\}$, the general Newton-Raphson Linearisation would give the following:

$$\Psi^n = \Psi^o + \frac{\partial \Psi^o}{\partial \Phi_1} (\Phi_1^n - \Phi_1^o) + \frac{\partial \Psi^o}{\partial \Phi_2} (\Phi_2^n - \Phi_2^o) + \frac{\partial \Psi^o}{\partial \Phi_3} (\Phi_3^n - \Phi_3^o) \quad (4.13)$$

The superscript ‘ n ’ refers to the current iteration and ‘ o ’ refers to the previous iteration.

4.2.4 Algebraic Equations

The coefficients of the algebraic equation are represented as follows:



Algebraic equations of all governing equations after discretisation are as follows:

- The liquid phase continuity equation, Equation (3.4), becomes:

$$A_{L,S}^{J,J} J_{L,S} + A_{L,P}^{J,U} U_{L,P} + A_{L,P}^{J,J} J_{L,P} + A_{L,P}^{J,\delta} \delta_P = B_{L,P}^J \quad (4.14)$$

- The liquid phase momentum equation, Equation (3.5), becomes:

$$A_{L,S}^{U,U} U_{L,S} + A_{L,S}^{U,J} J_{L,S} + A_{L,P}^{U,U} U_{L,P} + A_{L,P}^{U,J} J_{L,P} + A_{L,N}^{U,U} U_{L,N} + A_{L,P}^{U,\delta} \delta_P + A_{L,P}^{U,P} \left(\frac{dP}{d\chi} \right)_P = B_{L,P}^U \quad (4.15)$$

- The liquid phase energy equation, Equation (3.6), becomes:

$$A_{L,S}^{T,J} J_{L,S} + A_{L,S}^{T,T} T_{L,S} + A_{L,P}^{T,U} U_{L,P} + A_{L,P}^{T,J} J_{L,P} + A_{L,P}^{T,T} T_{L,P} + A_{L,N}^{T,T} T_{L,N} + A_{L,P}^{T,\delta} \delta_P = B_{L,P}^T \quad (4.16)$$

- The gas phase continuity equation, Equation (3.7), becomes:

$$A_{M,S}^{J,J} J_{M,S} + A_{M,P}^{J,U} U_{M,P} + A_{M,P}^{J,J} J_{M,P} + A_{M,P}^{J,\delta} \delta_P = B_{M,P}^J \quad (4.17)$$

- The gas phase momentum equation, Equation (3.8), becomes:

$$A_{M,S}^{U,U} U_{M,S} + A_{M,S}^{U,J} J_{M,S} + A_{M,P}^{U,U} U_{M,P} + A_{M,P}^{U,J} J_{M,P} + A_{M,N}^{U,U} U_{M,N} + A_{M,P}^{U,\delta} \delta_P + A_{M,P}^{U,P} \left(\frac{dP}{d\chi} \right)_P = B_{M,P}^U \quad (4.18)$$

- The gas phase energy equation, Equation (3.9), becomes:

$$A_{M,S}^{T,J} J_{M,S} + A_{M,S}^{T,T} T_{M,S} + A_{M,S}^{T,W_a} W_{a,S} + A_{M,P}^{T,U} U_{M,P} + A_{M,P}^{T,J} J_{M,P} + A_{M,P}^{T,T} T_{M,P} + A_{M,P}^{T,W_a} W_{a,P} + A_{M,N}^{T,T} T_{M,N} + A_{M,N}^{T,W_a} W_{a,N} + A_{M,P}^{T,\delta} \delta_P = B_{M,P}^T \quad (4.19)$$

- The gas phase mass fraction equation, Equation (3.10), becomes:

$$A_{M,S}^{W_a,J} J_{M,S} + A_{M,S}^{W_a,W_a} W_{a,S} + A_{M,P}^{W_a,U} U_{M,P} + A_{M,P}^{W_a,J} J_{M,P} + A_{M,P}^{W_a,W_a} W_{a,P} + A_{M,N}^{W_a,W_a} W_{a,N} + A_{M,P}^{W_a,\delta} \delta_P = B_{M,P}^{W_a} \quad (4.20)$$

The coefficients of the discretised equations in both phases are given in Appendix D of Siow [95].

Algebraic equations of the interface conditions are as follows:

- Discretisation and combination of velocity and shear continuity at the interface, Equation (3.11), leads to the following equation:

$$A_{\text{intf},S}^{U,U} U_{L,S} + A_{\text{intf},P}^{U,U} U_{M,P} + A_{\text{intf},N}^{U,U} U_{M,N} + A_{\text{intf},P}^{U,\delta} \delta_P = B_{\text{intf},P}^U \quad (4.21)$$

- The evaporated mass continuity equation, Equation (3.12), becomes:

$$A_{\text{intf},S}^{J,J} J_{L,S} + A_{\text{intf},P}^{J,J} J_{M,P} = B_{\text{intf},P}^J \quad (4.22)$$

- The temperature continuity equation, Equation (2.11), becomes:

$$A_{\text{intf},P}^{T,T} T_{M,P} + A_{\text{intf},P}^{T,W_a} W_{a,P} + A_{\text{intf},P}^{T,P} \left(\frac{dP}{d\chi} \right)_P = B_{\text{intf},P}^T \quad (4.23)$$

- The air impermeability equation, Equation (3.13), becomes:

$$A_{\text{intf},P}^{W_a,J} J_{M,P} + A_{\text{intf},P}^{W_a,W_a} W_{a,P} + A_{\text{intf},N}^{W_a,W_a} W_{a,N} + A_{\text{intf},P}^{W_a,\delta} \delta_P = B_{\text{intf},P}^{W_a} \quad (4.24)$$

- The energy continuity equation, Equation (3.14) becomes:

$$A_{\text{intf},S}^{\delta,T} T_{L,S} + A_{\text{intf},P}^{\delta,J} J_{M,P} + A_{\text{intf},P}^{\delta,T} T_{M,P} + A_{\text{intf},N}^{\delta,T} T_{M,N} + A_{\text{intf},P}^{\delta,\delta} \delta_P = B_{\text{intf},P}^{\delta} \quad (4.25)$$

The overall mass conservation, Equation (3.15) is approximated as the summation of the mass flows at east faces of each column of control volumes:

$$\sum_{jL=1}^{N_{y,L}-1} A_{L,jL}^{P,U} U_{L,jL} + \sum_{jG=1}^{N_{y,M}} A_{M,jG}^{P,U} U_{M,jG} + A_P^{P,\delta} \delta_P = B_P^P \quad (4.26)$$

The coefficients of Equations (4.21) to (4.26) are given in Appendix E of Siow [95]. This complete linearization introduces the following connections in the algebraic equations:

- between U , J , and δ in the continuity equations (Eqs. (4.14) and (4.17)),
- between U , J , dP/dx , and δ in the momentum equations (Eqs. (4.15) and (4.18)),
- between T , U , J , and δ in the liquid energy equation (Eq. (4.16)),
- between T , U , J , W , and δ in the mixture energy equation (Eq. (4.19)), and
- between W , U , J , and δ in the gas mass conservation equation (Eq. (4.20)).

4.2.5 Solution Method

Starting from an existing code for the condensation modeling, an in-house computer code was developed for the simulation of the evaporation phenomenon using Fortran 95 to compute the equation coefficients and solve the above set of linear algebraic equations. Starting at the first station, a full matrix is constructed using the discretised governing for the liquid region, the gas region, the interface conditions and the overall mass balance. The unknowns in the matrix are the variables U , J , T , W_a , and scalars δ and $dP/d\chi$. The U -momentum equations is solved for U , the continuity equation for J , the energy equation for T , the gas mass fraction equation for W_a , the interface energy continuity equation for δ and the global mass balance equation for $dP/d\chi$. Because the off-diagonal entries of the bordered block matrix are mainly zeros, it would be very inefficient to solve this matrix using a conventional technique such as Gauss elimination. In order to reduce the computation effort, a direct solver was developed based on the bordered matrix algorithm discussed by Behie et al. [99] and the standard block-tridiagonal matrix algorithm (BT-DMA). Because of non-linearities, an iterative approach is needed to arrive at a solution. The set is iterated to convergence at each axial station. The coupling and bordered matrix solution approach provide robust behaviour and fast convergence. A marching procedure is used starting from the inlet boundary conditions. Convergence of the solution is declared at each axial station when the relative change of all unknown values is less than 10^{-7} (described below). Computation proceeds along the channel until the marching reaches the end of the channel or the axial velocity becomes negative. The second condition may occur when opposing buoyancy forces are dominant.

The solution procedure is:

1. Form an initial guess of the dependent variables based on the inlet conditions.
2. Calculate local fluid properties based on the current air mass fraction and temperature fields.
3. Compute the coefficients of the discretized governing equations in both phases for the velocity, mass flux, temperature, and mass fraction, including interface and boundary conditions.

These coefficients form a block tri-diagonal matrix.

4. Compute the coefficients for the interface energy balance and the coefficients connecting the film thickness to all the field variables (via the Newton-Raphson linearizations). These coefficients form the vectors associated with the film thickness in the bordered matrix.
5. Compute the coefficients of the discretized overall mass conservation equation and the coefficients connecting the pressure gradient to the velocity equations. These coefficients form the vectors associated with the pressure gradient in the bordered matrix.
6. Perform a direct solution for all unknowns using a bordered matrix algorithm and a block TDMA [95].
7. Compare the current (new) solution to the previous iteration solution (old) at all control volumes and for the scalar quantities. The relative error of each dependent variable is calculated using:

$$E^{\Phi} = \left| \frac{\Phi^{\text{new}} - \Phi^{\text{old}}}{\Phi^{\text{new}}} \right| \quad (4.27)$$

If the relative error is higher than the convergence criterion, apply relaxation using:

$$\Phi = \Phi^{\text{new}} + \lambda^{\Phi}(\Phi^{\text{new}} - \Phi^{\text{old}}) \quad (4.28)$$

Typical values of the relaxation factors were 0.5, and 0.8 for T and W , respectively; no relaxation was used for U and J . Relaxation was used only to reduce the overall iteration count in some cases.

8. Repeat Steps 2 to 7 until a converged solution is reached at the axial station.
9. Progress to the next axial station using the converged solution from the previous station as an initial guess.
10. Repeat Steps 2 to 9 for the rest of the domain. Terminate computations if a negative value of U is found in a converged solution.

4.3 Discretisation of the Elliptic Model Governing Equations

In the elliptic model, a co-located variable storage scheme is applied, so that all the unknowns are located at the centre, P, of a typical non-orthogonal control volume as shown in Figure 4.1. The mass flow rate at each face of the control volume is determined by the face velocities. These velocities are determined at the integration point (ip) located at the centre of the face of the control volume (e, w, n, or s). Other fluxes are determined using the face value and gradient of the independent variables evaluated at the integration points. These fluxes are assumed constant along the face. Using the non-orthogonal grid results in a nine-point computational molecule, consisting of

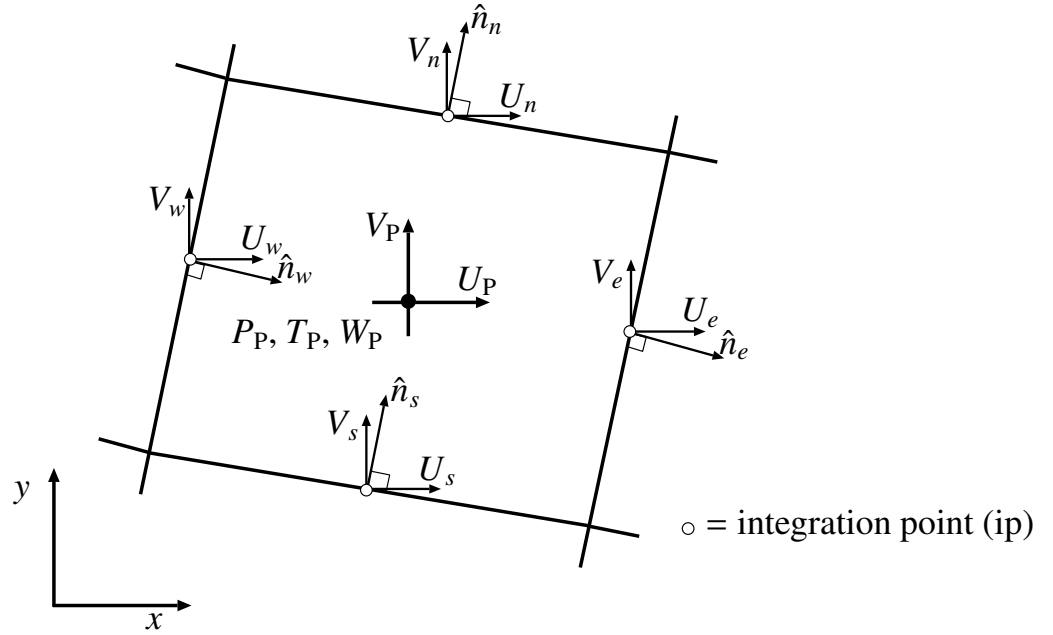


Figure 4.1: Co-located variable storage scheme.

the central node and its eight neighbouring nodes shown in Figure 3.4, for each field variable (U, V, P, T, and W) in both phases. The values at the corners of the control volume (ne, nw, se, and sw) are estimated by linear interpolation, Figure 3.5.

4.3.1 Algebraic Transport Equations

In this section, the details of the liquid phase governing equations discretisation are presented. The same methodology is applied to discretise the gas phase governing equations.

4.3.1.1 Liquid Phase Continuity Equation

The discretisation of Equation (2.20) yields to the following equation:

$$\begin{aligned} & \rho A_e (U_e n_{xe} + V_e n_{ye}) - \rho A_w (U_w n_{xw} + V_w n_{yw}) \\ & + \rho A_n (U_n n_{xn} + V_n n_{yn}) - \rho A_s (U_s n_{xs} + V_s n_{ys}) + \frac{\bar{V}_P (\rho_P - \rho_P^o)}{\Delta t} = 0 \end{aligned} \quad (4.29)$$

where U_e and V_e are face velocity components and n_{xe} and n_{ye} are the components of the normal unit vector on the east face. Note that the normal unit vector is outward on the east and north faces and inward on the west and south faces. In the development of the coupled algebraic equations, unsuperscripted variable represent values at the new time step; variables with “ o ” indicate the previous time step values. Equation (4.29) can be written as the balance of the mass flow rates as follows:

$$\dot{m}_e - \dot{m}_w + \dot{m}_n - \dot{m}_s + \frac{\bar{V}_P (\rho_P - \rho_P^o)}{\Delta t} = 0 \quad (4.30)$$

A pressure-weighted interpolation method (PWIM) based on the work of Rhie and Chow [100] is applied to estimate the face velocities. The PWIM estimations for the east and west face velocities are as follows. The estimation of the north and south face velocities follows the same procedure.

$$U_e = \mathcal{W}_e U_P + (1 - \mathcal{W}_e) U_E - \hat{d}_e^u \frac{\partial P}{\partial x} \Big|_e + \tilde{b}_e^u \quad (4.31)$$

$$U_w = \mathcal{W}_w U_W + (1 - \mathcal{W}_w) U_P - \hat{d}_w^u \frac{\partial P}{\partial x} \Big|_w + \tilde{b}_w^u \quad (4.32)$$

$$V_e = \mathcal{W}_e V_P + (1 - \mathcal{W}_e) V_E - \hat{d}_e^v \frac{\partial P}{\partial y} \Big|_e + \tilde{b}_e^v \quad (4.33)$$

$$V_w = \mathcal{W}_w V_W + (1 - \mathcal{W}_w) V_P - \hat{d}_w^v \frac{\partial P}{\partial y} \Big|_w + \tilde{b}_w^v \quad (4.34)$$

where $\mathcal{W}$ is a geometric linear interpolation at the face of the control volume and is defined as follows for the east and west faces:

$$\mathcal{W}_{e(i,j)} = \frac{\text{DISW}_{(i+1,j)}}{\text{DISE}_{(i,j)} + \text{DISW}_{(i+1,j)}} \quad (4.35)$$

$$\mathcal{W}_{w(i,j)} = \mathcal{W}_{e(i-1,j)} = \frac{\text{DISW}_{(i,j)}}{\text{DISE}_{(i-1,j)} + \text{DISW}_{(i,j)}} \quad (4.36)$$

and

$$\tilde{b}_e^u = \hat{d}_e^u \left\{ \mathcal{W}_e \frac{\partial P}{\partial x} \Big|_P^o + (1 - \mathcal{W}_e) \frac{\partial P}{\partial x} \Big|_E^o \right\} + \frac{\rho}{\Delta t} \hat{d}_e^u \left\{ U_e^o - [\mathcal{W}_e U_P^o + (1 - \mathcal{W}_e) U_E^o] \right\} \quad (4.37)$$

$$\tilde{b}_w^u = \hat{d}_w^u \left\{ \mathcal{W}_w \frac{\partial P}{\partial x} \Big|_W^o + (1 - \mathcal{W}_w) \frac{\partial P}{\partial x} \Big|_P^o \right\} + \frac{\rho}{\Delta t} \hat{d}_w^u \left\{ U_w^o - [\mathcal{W}_w U_W^o + (1 - \mathcal{W}_w) U_P^o] \right\} \quad (4.38)$$

$$\tilde{b}_e^v = \hat{d}_e^v \left\{ \mathcal{W}_e \frac{\partial P}{\partial y} \Big|_P^o + (1 - \mathcal{W}_e) \frac{\partial P}{\partial y} \Big|_E^o \right\} + \frac{\rho}{\Delta t} \hat{d}_e^v \left\{ V_e^o - [\mathcal{W}_e V_P^o + (1 - \mathcal{W}_e) V_E^o] \right\} \quad (4.39)$$

$$\tilde{b}_w^v = \hat{d}_w^v \left\{ \mathcal{W}_w \frac{\partial P}{\partial y} \Big|_W^o + (1 - \mathcal{W}_w) \frac{\partial P}{\partial y} \Big|_P^o \right\} + \frac{\rho}{\Delta t} \hat{d}_w^v \left\{ V_w^o - [\mathcal{W}_w V_W^o + (1 - \mathcal{W}_w) V_P^o] \right\} \quad (4.40)$$

$$\hat{d}_e^\phi = \mathbf{\Psi}_w \left\{ \frac{\mathcal{W}_e}{(a_P^{\phi,\phi})_P} + \frac{(1 - \mathcal{W}_e)}{(a_P^{\phi,\phi})_E} \right\} \quad (4.41)$$

$$\hat{d}_w^\phi = \mathbf{\Psi}_e \left\{ \frac{\mathcal{W}_w}{(a_P^{\phi,\phi})_W} + \frac{(1 - \mathcal{W}_w)}{(a_P^{\phi,\phi})_P} \right\} \quad (4.42)$$

In Equations (4.41) and (4.42), ϕ is u or v and $a_P^{\phi,\phi}$ is the nodal points coefficients in the U or V momentum equations. In order to compute the face volumes ($\mathbf{\Psi}_e$ and $\mathbf{\Psi}_w$), each control volume is

divided into quadrants by lines connecting the integration points e to w and n to s in Figure 3.7. The volume at an integration point is the summation of the volumes of the quadrants adjacent to the face. The pressure gradients at faces in Equations (4.31) to (4.34) are evaluated using the appropriate combination of co-ordinate derivatives $(\frac{\partial x}{\partial s}, \frac{\partial x}{\partial t}, \frac{\partial y}{\partial s}, \frac{\partial y}{\partial t})$ and derivatives of pressure in the $\hat{s}$ and $\hat{t}$ directions on a non-orthogonal grid. Using the chain rule and Cramer's rule, the derivatives in the x and y directions on face f are defined as follows:

$$\frac{\partial \Phi}{\partial x} \Big|_f = \mathcal{Y}_{t,f} \frac{\partial \Phi}{\partial s} \Big|_f - \mathcal{Y}_{s,f} \frac{\partial \Phi}{\partial t} \Big|_f \quad (4.43)$$

$$\frac{\partial \Phi}{\partial y} \Big|_f = \mathcal{X}_{s,f} \frac{\partial \Phi}{\partial t} \Big|_f - \mathcal{X}_{t,f} \frac{\partial \Phi}{\partial s} \Big|_f \quad (4.44)$$

where,

$$\mathcal{X}_{s,f} = \frac{\frac{\partial x}{\partial s} \Big|_f}{\left(\frac{\partial x}{\partial s} \Big|_f \frac{\partial y}{\partial t} \Big|_f - \frac{\partial x}{\partial t} \Big|_f \frac{\partial y}{\partial s} \Big|_f \right)} \quad (4.45)$$

$$\mathcal{X}_{t,f} = \frac{\frac{\partial x}{\partial t} \Big|_f}{\left(\frac{\partial x}{\partial s} \Big|_f \frac{\partial y}{\partial t} \Big|_f - \frac{\partial x}{\partial t} \Big|_f \frac{\partial y}{\partial s} \Big|_f \right)} \quad (4.46)$$

$$\mathcal{Y}_{s,f} = \frac{\frac{\partial y}{\partial s} \Big|_f}{\left(\frac{\partial x}{\partial s} \Big|_f \frac{\partial y}{\partial t} \Big|_f - \frac{\partial x}{\partial t} \Big|_f \frac{\partial y}{\partial s} \Big|_f \right)} \quad (4.47)$$

$$\mathcal{Y}_{t,f} = \frac{\frac{\partial y}{\partial t} \Big|_f}{\left(\frac{\partial x}{\partial s} \Big|_f \frac{\partial y}{\partial t} \Big|_f - \frac{\partial x}{\partial t} \Big|_f \frac{\partial y}{\partial s} \Big|_f \right)} \quad (4.48)$$

As shown in Figure 3.7, there are two direction vectors, $\hat{s}$ and $\hat{t}$, for each face and central node of the main control volume. The x and y derivatives for each face in Equations (4.43) and (4.44)

should be approximated using the nodal and corner values indicated as ne , nw , se , and sw in Figure 3.5:

$$\left. \frac{\partial \Phi}{\partial x} \right|_e = \frac{\mathcal{Y}_{t,e}}{(ds)_e} (\Phi_E - \Phi_P) - \frac{\mathcal{Y}_{s,e}}{(dt)_e} (\Phi_{ne} - \Phi_{se}) \quad (4.49)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_e = \frac{\mathcal{X}_{s,e}}{(dt)_e} (\Phi_{ne} - \Phi_{se}) - \frac{\mathcal{X}_{t,e}}{(ds)_e} (\Phi_E - \Phi_P) \quad (4.50)$$

$$\left. \frac{\partial \Phi}{\partial x} \right|_w = \frac{\mathcal{Y}_{t,w}}{(ds)_w} (\Phi_P - \Phi_W) - \frac{\mathcal{Y}_{s,w}}{(dt)_w} (\Phi_{nw} - \Phi_{sw}) \quad (4.51)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_w = \frac{\mathcal{X}_{s,w}}{(dt)_w} (\Phi_{nw} - \Phi_{sw}) - \frac{\mathcal{X}_{t,w}}{(ds)_w} (\Phi_P - \Phi_W) \quad (4.52)$$

$$\left. \frac{\partial \Phi}{\partial x} \right|_n = \frac{\mathcal{Y}_{t,n}}{(ds)_n} (\Phi_{ne} - \Phi_{nw}) - \frac{\mathcal{Y}_{s,n}}{(dt)_n} (\Phi_N - \Phi_P) \quad (4.53)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_n = \frac{\mathcal{X}_{s,n}}{(dt)_n} (\Phi_N - \Phi_P) - \frac{\mathcal{X}_{t,n}}{(ds)_n} (\Phi_{ne} - \Phi_{nw}) \quad (4.54)$$

$$\left. \frac{\partial \Phi}{\partial x} \right|_s = \frac{\mathcal{Y}_{t,s}}{(ds)_s} (\Phi_{se} - \Phi_{sw}) - \frac{\mathcal{Y}_{s,s}}{(dt)_s} (\Phi_P - \Phi_S) \quad (4.55)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_s = \frac{\mathcal{X}_{s,s}}{(dt)_s} (\Phi_P - \Phi_S) - \frac{\mathcal{X}_{t,s}}{(ds)_s} (\Phi_{se} - \Phi_{sw}) \quad (4.56)$$

The values at the control volume corners are calculated using a geometric interpolation in a non-uniform grid:

$$\Phi_{ne} = C_{ne1} \Phi_P + C_{ne2} \Phi_E + C_{ne3} \Phi_{NE} + C_{ne4} \Phi_N \quad (4.57)$$

$$\Phi_{nw} = C_{nw1} \Phi_W + C_{nw2} \Phi_P + C_{nw3} \Phi_N + C_{nw4} \Phi_{NW} \quad (4.58)$$

$$\Phi_{se} = C_{se1} \Phi_S + C_{se2} \Phi_{SE} + C_{se3} \Phi_E + C_{se4} \Phi_P \quad (4.59)$$

$$\Phi_{sw} = C_{sw1}\Phi_{SW} + C_{sw2}\Phi_S + C_{sw3}\Phi_P + C_{sw4}\Phi_W \quad (4.60)$$

where the numbering of C coefficients starts from 1 at the left bottom corner node and goes counter-clockwise around the control volume.

The nodal gradients of pressure in Equations (4.37) to (4.40) are calculated using the following equations:

$$\left. \frac{\partial \Phi}{\partial x} \right|_P = \frac{\mathcal{Y}_{t,P}}{(ds)_P} (\Phi_e - \Phi_w) - \frac{\mathcal{Y}_{s,P}}{(dt)_P} (\Phi_n - \Phi_s) \quad (4.61)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_P = \frac{\mathcal{X}_{s,P}}{(dt)_P} (\Phi_n - \Phi_s) - \frac{\mathcal{X}_{t,P}}{(ds)_P} (\Phi_e - \Phi_w) \quad (4.62)$$

The face values are computed by geometric interpolation using surrounding nodal values.

After substitution of Equations (4.57) to (4.60) into Equations (4.49) to (4.56) for variable P , the pressure gradients on the faces are approximated in terms of nodal pressure values. Now, the liquid continuity algebraic equation can be written in terms of nodal velocity and pressure values:

$$a_P^{c,p} P_P + \sum a_{NB8}^{c,p} P_{NB8} + a_P^{c,u} U_P + \sum a_{NB4}^{c,u} U_{NB4} + a_P^{c,v} V_P + \sum a_{NB4}^{c,v} V_{NB4} = b_P^c \quad (4.63)$$

The first and second superscripts of the a coefficients refer to the equation label and the multiplied variable, respectively. In summations, $NB4=\{E,W,N,S\}$ and $NB8=\{NB4,NE,NW,SE,SW\}$. The details of the summations are:

$$\sum a_{NB4}^{c,\phi} \Phi_{NB4} = a_E^{c,\phi} \Phi_E + a_W^{c,\phi} \Phi_W + a_N^{c,\phi} \Phi_N + a_S^{c,\phi} \Phi_S \quad (4.64)$$

and,

$$\sum a_{NB8}^{c,\phi} \Phi_{NB8} = \sum a_{NB4}^{c,\phi} \Phi_{NB4} + a_{NE}^{c,\phi} \Phi_{NE} + a_{NW}^{c,\phi} \Phi_{NW} + a_{SE}^{c,\phi} \Phi_{SE} + a_{SW}^{c,\phi} \Phi_{SW} \quad (4.65)$$

Therefore, discretisation of the continuity equation produces implicit connections between five U nodes, five V nodes, and nine P nodes. The coefficients of the liquid continuity equation are given in Appendix D, Section D.1.

4.3.1.2 Liquid Phase x -momentum Equation

Equation (2.21) yields to the following algebraic equation for x -momentum:

$$\begin{aligned} \frac{(\rho_P \mathcal{V}_P)}{\Delta t} (U_P - U_P^o) + \dot{m}_e U_e - \dot{m}_w U_w + \dot{m}_n U_n - \dot{m}_s U_s = \\ - \frac{\partial P}{\partial x} \Big|_P + \rho_P g_x \mathcal{V}_P + D_e^u \frac{\partial U}{\partial n} \Big|_e - D_w^u \frac{\partial U}{\partial n} \Big|_w + D_n^u \frac{\partial U}{\partial n} \Big|_n - D_s^u \frac{\partial U}{\partial n} \Big|_s \end{aligned} \quad (4.66)$$

In Equation (4.66), $D_f^u = \mu_f A_f$ and mass flow rates from the previous time step ($\dot{m}_f^o$) are used for $\dot{m}$ values in the advection terms. The faces U velocities are approximated in terms of nodal values using the convective weight coefficient α_f at each face and an algebraic approximation to the exponential differencing scheme by Raithby and Schneider [101]:

$$\Phi_e = (0.5 + \alpha_e) \Phi_P + (0.5 - \alpha_e) \Phi_E \quad (4.67)$$

$$\Phi_w = (0.5 + \alpha_w) \Phi_W + (0.5 - \alpha_w) \Phi_P \quad (4.68)$$

$$\Phi_n = (0.5 + \alpha_n) \Phi_P + (0.5 - \alpha_n) \Phi_N \quad (4.69)$$

$$\Phi_s = (0.5 + \alpha_s) \Phi_S + (0.5 - \alpha_s) \Phi_P \quad (4.70)$$

α_f values are computed as a function of the local ratio of advective to diffusive transport rates:

$$\alpha_f = \text{sign}(\dot{m}_f) \frac{0.5 \text{Pe}_f^2}{5 + \text{Pe}_f^2} \quad (4.71)$$

$$\text{Pe}_f = \frac{\dot{m}_f}{D_f} \quad (4.72)$$

The normal derivative of U velocity at the east and north faces is defined as:

$$\frac{\partial U}{\partial n} \Big|_e = \beta_e \frac{\frac{\partial U}{\partial s} \Big|_e - (\hat{s}_e \cdot \hat{t}_e) \frac{\partial U}{\partial t} \Big|_e}{\hat{n}_e \cdot \hat{s}_e} \quad (4.73)$$

$$\left. \frac{\partial U}{\partial n} \right|_n = \beta_n \frac{-(\hat{s}_n \cdot \hat{t}_n) \left. \frac{\partial U}{\partial s} \right|_n + \left. \frac{\partial U}{\partial t} \right|_n}{\hat{t}_n \cdot \hat{n}_n} \quad (4.74)$$

where β_f is the diffusion weighting coefficient and defined as follows:

$$\beta_f = \frac{1 + 0.005 \text{Pe}_f^2}{1 + 0.05 \text{Pe}_f^2} \quad (4.75)$$

The gradients at the east and north faces are:

$$\left. \frac{\partial U}{\partial s} \right|_e = \frac{U_E - U_P}{(ds)_e}, \quad \left. \frac{\partial U}{\partial t} \right|_e = \frac{U_{ne} - U_{se}}{(dt)_e} \quad (4.76)$$

$$\left. \frac{\partial U}{\partial s} \right|_n = \frac{U_{ne} - U_{nw}}{(ds)_n}, \quad \left. \frac{\partial U}{\partial t} \right|_n = \frac{U_N - U_P}{(dt)_n} \quad (4.77)$$

U_{ne} , U_{nw} , and U_{se} are approximated using Equations (4.57) to (4.59), respectively.

Following the discretisation procedure explained above, the final form of the linearised U -momentum equation is:

$$a_P^{u,u} U_P + \sum a_{\text{NB8}}^{u,u} U_{\text{NB8}} + a_P^{u,p} P_P + \sum a_{\text{NB4}}^{u,p} P_{\text{NB4}} = b_P^u \quad (4.78)$$

The coefficients of the U -momentum equation are given in Appendix D, Section D.2.

4.3.1.3 Liquid Phase y-momentum Equation

The discretisation of Equation (2.22) yields to the following equation:

$$\begin{aligned} \frac{(\rho_P \bar{V}_P)}{\Delta t} (V_P - V_P^o) + \dot{m}_e V_e - \dot{m}_w V_w + \dot{m}_n V_n - \dot{m}_s V_s = \\ - \left. \frac{\partial P}{\partial y} \right|_P \bar{V}_P + D_e^v \left. \frac{\partial V}{\partial n} \right|_e - D_w^v \left. \frac{\partial V}{\partial n} \right|_w + D_n^v \left. \frac{\partial V}{\partial n} \right|_n - D_s^v \left. \frac{\partial V}{\partial n} \right|_s \end{aligned} \quad (4.79)$$

where $D_f^u = \mu_f A_f$. Equation (4.79) is discretised in the same manner as was used for the x -momentum equation:

$$a_P^{v,v} V_P + \sum a_{\text{NB8}}^{v,v} V_{\text{NB8}} + a_P^{v,p} P_P + \sum a_{\text{NB4}}^{v,p} P_{\text{NB4}} = b_P^v \quad (4.80)$$

The coefficients of the V -momentum equation are given in Appendix D, Section D.3.

4.3.1.4 Liquid Phase Energy Equation

Equation (2.23) yields to the following equation for conservation of energy in the liquid phase:

$$\begin{aligned} \frac{(\rho_P C_{PP} \Psi_P)}{\Delta t} (T_P - T_P^o) + \dot{m}_e [C_{Pe} T_e + W_{Se} (\bar{h}_S - \bar{h}_W)_e] - \dot{m}_w [C_{Pw} T_w + W_{Sw} (\bar{h}_S - \bar{h}_W)_w] \\ + \dot{m}_n [C_{Pn} T_n + W_{Sn} (\bar{h}_S - \bar{h}_W)_n] - \dot{m}_s [C_{Ps} T_s + W_{Ss} (\bar{h}_S - \bar{h}_W)_s] = \\ D_e^t \frac{\partial T}{\partial n} \Big|_e - D_w^t \frac{\partial T}{\partial n} \Big|_w + D_n^t \frac{\partial T}{\partial n} \Big|_n - D_s^t \frac{\partial T}{\partial n} \Big|_s + \tilde{D}_e^t \frac{\partial W_S}{\partial n} \Big|_e - \tilde{D}_w^t \frac{\partial W_S}{\partial n} \Big|_w + \tilde{D}_n^t \frac{\partial W_S}{\partial n} \Big|_n - \tilde{D}_s^t \frac{\partial W_S}{\partial n} \Big|_s \end{aligned} \quad (4.81)$$

where $D_f^t = k_f A_f$ and $\tilde{D}_f^t = \rho_f D_f^{AB} A_f (\bar{h}_S - \bar{h}_W)_f$. Discretisation of Equation (4.81) yields to:

$$a_P^{t,t} T_P + \sum a_{NB8}^{t,t} T_{NB8} + a_P^{t,\xi} W_{SP} + \sum a_{NB8}^{t,\xi} W_{SNB8} = b_P^t \quad (4.82)$$

The mass fraction coefficients and the right hand side of Equation (4.82) are given in Appendix D, Section D.4.

4.3.1.5 Liquid Phase Mass Fraction Equation

Equation (2.24) yields to the following equation for conservation of mass in the liquid:

$$\begin{aligned} \frac{(\rho_P \Psi_P)}{\Delta t} (W_{SP} - W_{SP}^o) + \dot{m}_e W_{Se} - \dot{m}_w W_{Sw} + \dot{m}_n W_{Sn} - \dot{m}_s W_{Ss} = \\ D_e^w \frac{\partial W_S}{\partial n} \Big|_e - D_w^w \frac{\partial W_S}{\partial n} \Big|_w + D_n^w \frac{\partial W_S}{\partial n} \Big|_n - D_s^w \frac{\partial W_S}{\partial n} \Big|_s \end{aligned} \quad (4.83)$$

where $D_f^w = \rho_f D_f^{AB}$. Discretisation of Equation (4.83) yields to:

$$a_P^{w,w} W_{SP} + \sum a_{NB8}^{w,w} W_{SNB8} = b_P^w \quad (4.84)$$

The derivations of $a_P^{w,w}$ and $a_{NB8}^{w,w}$ are analogous to those for the U velocity coefficients in x -momentum equation using $\rho_f D_f^{AB}$ instead of μ_f .

4.3.2 Algebraic Interface Equations

At the liquid-gas interface, one equation is required to form an algebraic equation for each of the field variables at either the liquid or gas side. In these algebraic equations, the nodes on both liquid and gas sides of the interface along with the adjacent nodes in both regions are involved. Figure 4.2 shows the indexing notation of the interface nodes and their neighbouring control volumes. This naming system is applied to all the algebraic form of the interface equations.

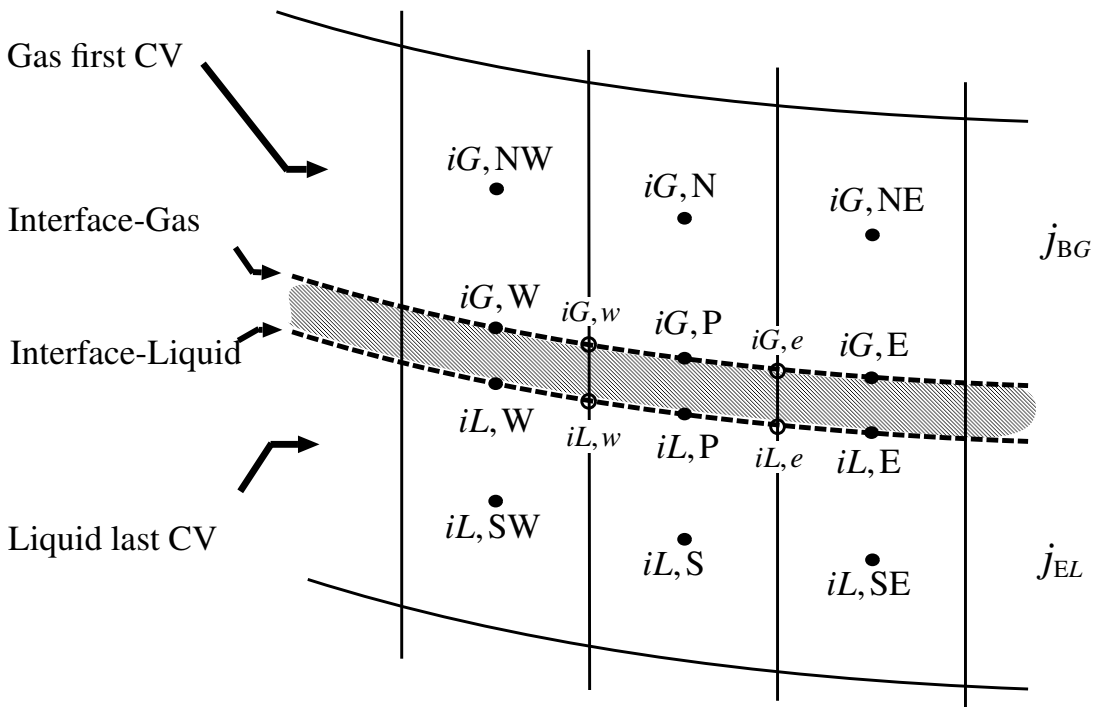


Figure 4.2: Indexing notation for interface and neighbouring control volumes; the spacing between the nodes at the interface is exaggerated for illustration purposes.

4.3.2.1 Normal Force Balance

The normal force balance, Equation (2.30), is used as an equation for P on the liquid interface ($j = j_{EL} + 1$). The 2D stress tensor τ is defined in terms of the normal and shear stress:

$$\tau = \begin{pmatrix} \tau_{xx} & \tau_{yx} \\ \tau_{xy} & \tau_{yy} \end{pmatrix} \quad (4.85)$$

For incompressible fluids, the stress tensor can be written in the compact form of:

$$\tau_{ij} = -P \delta_{ij} + \mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (4.86)$$

where i and j refer to the coordinates x and y and δ_{ij} in the index notation is the Kronecker delta. Substitution of Equation (4.85) in Equation (2.30) results in the following equation:

$$\left(\tau_{xx} n_x^2 + 2 \tau_{xy} n_x n_y + \tau_{yy} n_y^2 \right)_{L,intf} + \sigma K = \left(\tau_{xx} n_x^2 + 2 \tau_{xy} n_x n_y + \tau_{yy} n_y^2 \right)_{G,intf} \quad (4.87)$$

Substitution of all stresses in Equation (4.87) results in:

$$\begin{aligned} \left(-P + 2 \mu \left(\frac{\partial U}{\partial x} \right) n_x^2 + 2 \mu \left(\frac{\partial U}{\partial r} + \frac{\partial V}{\partial x} \right) n_x n_y + 2 \mu \left(\frac{\partial V}{\partial y} \right) n_y^2 \right)_{L,intf} + \sigma K = \\ \left(-P + 2 \mu \left(\frac{\partial U}{\partial x} \right) n_x^2 + 2 \mu \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) n_x n_y + 2 \mu \left(\frac{\partial V}{\partial y} \right) n_y^2 \right)_{G,intf} \end{aligned} \quad (4.88)$$

The velocity derivatives are evaluated based on central differencing scheme. One-dimensional interpolation is employed to determine the corner values (U_{ne} and U_{nw}) for the liquid side of the interface and (U_{se} and U_{sw}) for the gas side of the interface from its interfacial two neighbours. For example, U_{ne} at the liquid side of the interface is determined by ($U_{ne} = f_{ne} U_N + (1 - f_{ne}) U_{NE}$) where f_{ne} is a linear interpolation factor based on the grid spacing. The derivatives at the interface for any transport variable can be given in general forms by the following expressions:

$$\left. \frac{\partial \Phi}{\partial x} \right|_{L,intf} = \left(\frac{\partial \Phi}{\partial x} \right)_{iL,S} = A_{x1} \Phi_{iL,S} + A_{x2} \Phi_{iL,P} + A_{x3} \Phi_{iL,E} + A_{x4} \Phi_{iL,W} \quad (4.89)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_{L,intf} = \left(\frac{\partial \Phi}{\partial y} \right)_{iL,S} = A_{y1} \Phi_{iL,S} + A_{y2} \Phi_{iL,P} + A_{y3} \Phi_{iL,E} + A_{y4} \Phi_{iL,W} \quad (4.90)$$

$$\left. \frac{\partial \Phi}{\partial x} \right|_{G,\text{intf}} = \left(\frac{\partial \Phi}{\partial x} \right)_s \Big|_{iG,N} = B_{x1} \Phi_{iG,N} + B_{x2} \Phi_{iG,P} + B_{x3} \Phi_{iG,E} + B_{x4} \Phi_{iG,W} \quad (4.91)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_{G,\text{intf}} = \left(\frac{\partial \Phi}{\partial y} \right)_s \Big|_{iG,N} = B_{y1} \Phi_{iG,N} + B_{y2} \Phi_{iG,P} + B_{y3} \Phi_{iG,E} + B_{y4} \Phi_{iG,W} \quad (4.92)$$

For the purpose of brevity, the liquid and the gas interfaces are shown with iL and iG , respectively in the interface algebraic equations. iL,S and iG,N are the last and first control volumes in the liquid and gas phases, respectively. The coefficients in Equations (4.89) to (4.92) are:

$$\begin{aligned} A_{x1} &= \frac{1}{\Psi_n} \left[\frac{s_{yn}}{(dt)_n} \right]_{iL,S} & A_{x2} &= \frac{1}{\Psi_n} \left[\frac{t_{yn}}{(ds)_n} (f_{ne} - (1 - f_{nw})) - \frac{s_{yn}}{(dt)_n} \right]_{iL,S} \\ A_{x3} &= \frac{1}{\Psi_n} \left[\frac{t_{yn}}{(ds)_n} (1 - f_{ne}) \right]_{iL,S} & A_{x4} &= -\frac{1}{\Psi_n} \left[\frac{t_{yn}}{(ds)_n} f_{nw} \right]_{iL,S} \end{aligned} \quad (4.93)$$

$$\begin{aligned} A_{y1} &= -\frac{1}{\Psi_n} \left[\frac{s_{xn}}{(dt)_n} \right]_{iL,S} & A_{y2} &= \frac{1}{\Psi_n} \left[\frac{s_{xn}}{(dt)_n} - \frac{t_{xn}}{(ds)_n} (f_{ne} - (1 - f_{nw})) \right]_{iL,S} \\ A_{y3} &= -\frac{1}{\Psi_n} \left[\frac{t_{xn}}{(ds)_n} (1 - f_{ne}) \right]_{iL,S} & A_{y4} &= \frac{1}{\Psi_n} \left[\frac{t_{xn}}{(ds)_n} f_{nw} \right]_{iL,S} \end{aligned} \quad (4.94)$$

$$\begin{aligned} B_{x1} &= -\frac{1}{\Psi_s} \left[\frac{s_{ys}}{(dt)_s} \right]_{iG,N} & B_{x2} &= \frac{1}{\Psi_s} \left[\frac{t_{ys}}{(ds)_s} (f_{se} - (1 - f_{sw})) + \frac{s_{ys}}{(dt)_s} \right]_{iG,N} \\ B_{x3} &= \frac{1}{\Psi_s} \left[\frac{t_{ys}}{(ds)_s} (1 - f_{se}) \right]_{iG,N} & B_{x4} &= -\frac{1}{\Psi_s} \left[\frac{t_{ys}}{(ds)_s} f_{sw} \right]_{iG,N} \end{aligned} \quad (4.95)$$

$$\begin{aligned} B_{y1} &= \frac{1}{\Psi_s} \left[\frac{s_{xs}}{(dt)_s} \right]_{iG,N} & B_{y2} &= \frac{1}{\Psi_s} \left[\frac{-s_{xs}}{(dt)_s} - \frac{t_{xs}}{(ds)_s} (f_{se} - (1 - f_{sw})) \right]_{iG,N} \\ B_{y3} &= -\frac{1}{\Psi_s} \left[\frac{t_{xs}}{(ds)_s} (1 - f_{se}) \right]_{iG,N} & B_{y4} &= \frac{1}{\Psi_s} \left[\frac{t_{xs}}{(ds)_s} f_{sw} \right]_{iG,N} \end{aligned} \quad (4.96)$$

The geometrical terms, Ψ_n and Ψ_s , are defined as:

$$\Psi_n = (s_{xn} t_{yn} - t_{xn} s_{yn})_{iL,S} \quad \Psi_s = (s_{xs} t_{ys} - t_{xs} s_{ys})_{iG,N} \quad (4.97)$$

Applying the velocity gradient definitions, Equation (4.88) can be written as:

$$\begin{aligned}
 & -P_{iL} + 2 \left(\mu n_x^2 \right)_{iL,P} (A_{x1} U_{iL,S} + A_{x2} U_{iL,P} + A_{x3} U_{iL,E} + A_{x4} U_{iL,W}) \\
 & + 2 \left(\mu n_x n_y \right)_{iL,P} (A_{y1} U_{iL,S} + A_{y2} U_{iL,P} + A_{y3} U_{iL,E} + A_{y4} U_{iL,W}) \\
 & + 2 \left(\mu n_x n_y \right)_{iL,P} (A_{x1} V_{iL,S} + A_{x2} V_{iL,P} + A_{x3} V_{iL,E} + A_{x4} V_{iL,W}) \\
 & + 2 \left(\mu n_y^2 \right)_{iL,P} (A_{y1} V_{iL,S} + A_{y2} V_{iL,P} + A_{y3} V_{iL,E} + A_{y4} V_{iL,W}) + \sigma K = \\
 & -P_{iG} + 2 \left(\mu n_x^2 \right)_{iG,P} (B_{x1} U_{iG,N} + B_{x2} U_{iG,P} + B_{x3} U_{iG,E} + B_{x4} U_{iG,W}) \\
 & + 2 \left(\mu n_x n_y \right)_{iG,P} (B_{y1} U_{iG,N} + B_{y2} U_{iG,P} + B_{y3} U_{iG,E} + B_{y4} U_{iG,W}) \\
 & + 2 \left(\mu n_x n_y \right)_{iG,P} (B_{x1} V_{iG,N} + B_{x2} V_{iG,P} + B_{x3} V_{iG,E} + B_{x4} V_{iG,W}) \\
 & + 2 \left(\mu n_y^2 \right)_{iG,P} (B_{y1} V_{iG,N} + B_{y2} V_{iG,P} + B_{y3} V_{iG,E} + B_{y4} V_{iG,W})
 \end{aligned} \tag{4.98}$$

The final form of the normal force balance algebraic equation to calculate the liquid interface pressure is:

$$\begin{aligned}
 & a_{iL,P}^{c,p} P_{iL,P} + a_{iL,N}^{c,p} P_{iG,P} + a_{iL,P}^{c,u} U_{iL,P} + a_{iL,E}^{c,u} U_{iL,E} + a_{iL,W}^{c,u} U_{iL,W} + a_{iL,S}^{c,u} U_{iL,S} + \\
 & a_{iL,P}^{c,v} V_{iL,P} + a_{iL,E}^{c,v} V_{iL,E} + a_{iL,W}^{c,v} V_{iL,W} + a_{iL,S}^{c,v} V_{iL,S} + a_{iL,N}^{c,u} U_{iG,P} + a_{iL,NE}^{c,u} U_{iG,E} + \\
 & a_{iL,NW}^{c,u} U_{iG,W} + a_{iL,N}^{c,v} V_{iG,P} + a_{iL,NE}^{c,v} V_{iG,E} + a_{iL,NW}^{c,v} V_{iG,W} = b_{iL,P}^c \tag{4.99}
 \end{aligned}$$

The coefficients of Equation (4.99) are given in Appendix E, Section E.1. In this work, the surface tension force is omitted.

4.3.2.2 Zero Pressure Gradient

This condition is employed on the gas interface ($j = j_{BG} - 1$) to govern the pressure $P_{iG,P}$. Discretisation of Equation (2.38) leads to the algebraic form as follows:

$$\begin{aligned}
 \left. \frac{\partial P}{\partial n} \right|_{iG,P} &= (B_{x2} P_{iG,P} + B_{x3} P_{iG,E} + B_{x4} P_{iG,W} + B_{x1} P_{iG,N}) n_{xs}|_{iG,N} + \\
 & (B_{y2} P_{iG,P} + B_{y3} P_{iG,E} + B_{y4} P_{iG,W} + B_{y1} P_{iG,N}) n_{ys}|_{iG,N} = 0 \tag{4.100}
 \end{aligned}$$

which leads to:

$$a_{iG,P}^{c,p} P_{iG,P} + a_{iG,N}^{c,p} P_{iG,N} + a_{iG,W}^{c,p} P_{iG,W} + a_{iG,E}^{c,p} P_{iG,E} = 0 \quad (4.101)$$

The coefficients of Equation (4.101) are given in Appendix E, Section E.2.

4.3.2.3 Tangential Force Balance

The algebraic tangential force balance condition is used for the calculation of gas interface velocity, $U_{iG,P}$. Equation (2.31) can be written in terms of the normal and shear stresses at the interface as follows:

$$\left(\tau_{xx} n_x s_x + \tau_{xy} (n_y s_x + n_x s_y) + \tau_{yy} n_y s_y \right)_{L,\text{intf}} - \frac{\partial \sigma}{\partial s} \Big|_{L,\text{intf}} = \left(\tau_{xx} n_x s_x + \tau_{xy} (n_y s_x + n_x s_y) + \tau_{yy} n_y s_y \right)_{G,\text{intf}} \quad (4.102)$$

Equation (4.102) can be expressed in terms of velocity gradients:

$$\begin{aligned} \left(2 \mu \left(\frac{\partial U}{\partial x} \right) n_x s_x + \mu \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) (n_y s_x + n_x s_y) + 2 \mu \left(\frac{\partial V}{\partial y} \right) n_y s_y \right)_{L,\text{intf}} - \frac{\partial \sigma}{\partial s} \Big|_{L,\text{intf}} = \\ \left(2 \mu \left(\frac{\partial U}{\partial x} \right) n_x s_x + \mu \left(\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) (n_y s_x + n_x s_y) + 2 \mu \left(\frac{\partial V}{\partial y} \right) n_y s_y \right)_{G,\text{intf}} \end{aligned} \quad (4.103)$$

Using the Equations (4.89) to (4.92), Equation (4.103) can be simplified as follows:

$$\begin{aligned}
 & 2 (\mu n_x s_x)_{iL,P} (A_{x1} U_{iL,S} + A_{x2} U_{iL,P} + A_{x3} U_{iL,E} + A_{x4} U_{iL,W}) \\
 & + \left[\mu (n_y s_x + n_x s_y) \right]_{iL,P} (A_{y1} U_{iL,S} + A_{y2} U_{iL,P} + A_{y3} U_{iL,E} + A_{y4} U_{iL,W}) \\
 & + \left[\mu (n_y s_x + n_x s_y) \right]_{iL,P} (A_{x1} V_{iL,S} + A_{x2} V_{iL,P} + A_{x3} V_{iL,E} + A_{x4} V_{iL,W}) \\
 & + 2 (\mu n_y s_y)_{iL,P} (A_{y1} V_{iL,S} + A_{y2} V_{iL,P} + A_{y3} V_{iL,E} + A_{y4} V_{iL,W}) - \frac{\partial \sigma}{\partial s} \Big|_{L, \text{intf}} = \\
 & 2 (\mu n_x s_x)_{iG,P} (B_{x1} U_{iG,N} + B_{x2} U_{iG,P} + B_{x3} U_{iG,E} + B_{x4} U_{iG,W}) \\
 & + \left[\mu (n_y s_x + n_x s_y) \right]_{iG,P} (B_{y1} U_{iG,N} + B_{y2} U_{iG,P} + B_{y3} U_{iG,E} + B_{y4} U_{iG,W}) \\
 & + \left[\mu (n_y s_x + n_x s_y) \right]_{iG,P} (B_{x1} V_{iG,N} + B_{x2} V_{iG,P} + B_{x3} V_{iG,E} + B_{x4} V_{iG,W}) \\
 & + 2 (\mu n_y s_y)_{iG,P} (B_{y1} V_{iG,N} + B_{y2} V_{iG,P} + B_{y3} V_{iG,E} + B_{y4} V_{iG,W})
 \end{aligned} \tag{4.104}$$

The algebraic equation for tangential force balance that is used to calculate the $U_{iG,P}$ at the gas interface can be written as:

$$\begin{aligned}
 & a_{iG,P}^{u,u} U_{iG,P} + a_{iG,E}^{u,u} U_{iG,E} + a_{iG,W}^{u,u} U_{iG,W} + a_{iG,N}^{u,u} U_{iG,N} + \\
 & a_{iG,P}^{u,v} V_{iG,P} + a_{iG,E}^{u,v} V_{iG,E} + a_{iG,W}^{u,v} V_{iG,W} + a_{iG,N}^{u,v} V_{iG,N} + a_{iG,S}^{u,u} U_{iL,P} + a_{iG,SE}^{u,u} U_{iL,E} + \\
 & a_{iG,SW}^{u,u} U_{iL,W} + a_{iG,S}^{u,v} V_{iL,P} + a_{iG,SE}^{u,v} V_{iL,E} + a_{iG,SW}^{u,v} V_{iL,W} = b_{iG,P}^u \tag{4.105}
 \end{aligned}$$

The coefficients of Equation (4.105) are given in Appendix E, Section E.3. In this work, $\frac{\partial \sigma}{\partial s} = 0$

4.3.2.4 Tangential Velocity Equality

The continuity of tangential velocity at the interface, Equation (2.32), can be written based on the velocity and tangent vectors and used to calculate $U_{iL,P}$:

$$(U \hat{i} + V \hat{j})_{iG} \cdot (s_x \hat{i} + s_y \hat{j})_{iG} = (U \hat{i} + V \hat{j})_{iL} \cdot (s_x \hat{i} + s_y \hat{j})_{iL} \tag{4.106}$$

The algebraic form of Equation (4.106) is:

$$a_{iL,P}^{u,u} U_{iL,P} + a_{iL,N}^{u,u} U_{iG,P} + a_{iL,P}^{u,v} V_{iL,P} + a_{iL,N}^{u,v} V_{iG,P} = 0 \quad (4.107)$$

The coefficients of Equation (4.107) are given in Appendix E, Section E.4.

4.3.2.5 Continuity of Mass at the Interface

Equation (2.33) is used to calculate $V_{iG,P}$. Continuity of mass at the interface can be written as:

$$\left(\rho A \vec{V} \cdot \hat{n} \right)_{iL,P} = \left(\rho A \vec{V} \cdot \hat{n} \right)_{iG,P} \quad (4.108)$$

Simple calculation of the dot product results in:

$$a_{iG,P}^{v,u} U_{iG,P} + a_{iG,S}^{v,u} U_{iL,P} + a_{iG,P}^{v,v} V_{iG,P} + a_{iG,S}^{v,v} V_{iL,P} = 0 \quad (4.109)$$

The coefficients of Equation (4.109) are given in Appendix E, Section E.5.

4.3.2.6 Continuity of Energy at the Interface

The energy continuity at the interface, Equation (2.34), is used as the governing equation for $V_{iL,P}$.

This equation can be written in terms of velocity and normal unit vectors as:

$$\left(\rho A \vec{V} \cdot \hat{n} \right)_{iL,P} = \dot{m}_{\text{intf}} = \frac{A_{iL,P}}{h_{fg}} \left(-k_{iL,P} \frac{\partial T}{\partial n} \Big|_{iL,P} + k_{iG,P} \frac{\partial T}{\partial n} \Big|_{iG,P} \right) \quad (4.110)$$

Applying previous approaches for the evaluation of the gradients and calculation of dot product of vectors gives the algebraic form of Equation (4.110) as:

$$a_{iL,P}^{v,u} U_{iL,P} + a_{iL,P}^{v,v} V_{iL,P} + a_{iL,P}^{v,t} T_{iL,P} + a_{iL,E}^{v,t} T_{iL,E} + a_{iL,W}^{v,t} T_{iL,W} + \\ a_{iL,S}^{v,t} T_{iL,S} + a_{iL,N}^{v,t} T_{iG,P} + a_{iL,NE}^{v,t} T_{iG,E} + a_{iL,NW}^{v,t} T_{iG,W} = b_{iL,P}^v \quad (4.111)$$

The coefficients of Equation (4.111) are given in Appendix E, Section E.6.

4.3.2.7 Equilibrium Condition at the Interface

The gas-liquid interface obeys the equilibrium condition described by Equation (2.35). The equilibrium temperature is a function of the salt mass fraction, mixture pressure and air mass fraction at the interface ($T_{iL} = F(W_{iL}, P_{iG}, W_{iG})$). The equilibrium temperature function, described in Appendix C, can be written as follows using the Newton-Raphson linearisation:

$$T_{iL} = T_{iL}^o + \frac{\partial F}{\partial W_{iL}} (W_{iL} - W_{iL}^o) + \frac{\partial F}{\partial P_{iG}} (P_{iG} - P_{iG}^o) + \frac{\partial F}{\partial W_{iG}} (W_{iG} - W_{iG}^o) \quad (4.112)$$

The liquid interface temperature, $T_{iL,P}$, algebraic equation is:

$$a_{iL,P}^{t,t} T_{iL,P} + a_{iL,P}^{t,w} W_{iL,P} + a_{iG,P}^{t,p} P_{iG,P} + a_{iG,P}^{t,w} W_{iG,P} = b_{iL,P}^t \quad (4.113)$$

The coefficients of Equation (4.113) are given in Appendix E, Section E.7.

4.3.2.8 Temperature Equality at the Interface

The gas phase interface temperature equation is the equality of $T_{iG,P}$ and $T_{iL,P}$. The algebraic equation for $T_{iG,P}$ is as follows:

$$a_{iG,P}^{t,t} T_{iG,P} + a_{iG,S}^{t,t} T_{iL,P} = 0 \quad (4.114)$$

The coefficients of Equation (4.114) are given in Appendix E, Section E.8.

4.3.2.9 Impermeability of Gas

Equation (2.36) has an inter-equation coupling term ($\dot{m}_{\text{intf}} W_a$). This term includes the velocity components and gas mass fraction on the interface. Therefore, it needs to be linearised using the Newton-Raphson method:

$$\dot{m}_{\text{intf}} W_a = (\rho A n_x)_{iG,P} [U W^o + U^o W - U^o W^o]_{iG,P} + (\rho A n_y)_{iG,P} [V W^o + V^o W - V^o W^o]_{iG,P} \quad (4.115)$$

Applying the same approach for the approximation of the gradient term in Equation (2.36) and use of Equation (4.115) result in the algebraic form of the impermeability equation:

$$a_{iG,P}^{w,w} W_{iG,P} + a_{iG,E}^{w,w} W_{iG,E} + a_{iG,W}^{w,w} W_{iG,W} + a_{iG,N}^{w,w} W_{iG,N} + a_{iG,P}^{w,u} U_{iG,P} + a_{iG,P}^{w,v} V_{iG,P} = b_{iG,P}^w \quad (4.116)$$

The coefficients of Equation (4.116) are given in Appendix E, Section E.9.

4.3.2.10 Impermeability of Salt

Newton-Raphson linearisation is applied to $(\dot{m}_{\text{intf}} W_S)$ term in Equation (2.37).

$$\dot{m}_{\text{intf}} W_S = (\rho A n_x)_{iL,P} [U W^o + U^o W - U^o W^o]_{iL,P} + (\rho A n_y)_{iL,P} [V W^o + V^o W - V^o W^o]_{iL,P} \quad (4.117)$$

By Applying Equation (4.117) and the approximation of the gradient term, the W_S interface linear equation is formed:

$$a_{iL,P}^{w,w} W_{iL,P} + a_{iL,E}^{w,w} W_{iL,E} + a_{iL,W}^{w,w} W_{iL,W} + a_{iL,S}^{w,w} W_{iL,S} + a_{iL,P}^{w,u} U_{iL,P} + a_{iL,P}^{w,v} V_{iL,P} = b_{iL,P}^w \quad (4.118)$$

The coefficients of Equation (4.118) are given in Appendix E, Section E.10.

4.3.3 Boundary Condition Equation Implementation

Boundary conditions are imposed by means of utilizing zero-width boundary control volumes. The boundary integration points are located at the centre of the face of these control volumes. A linear algebraic equation is used to define the boundary nodal value. When the coefficients of the linear equation are determined so that they prescribe the required boundary condition, these linear equations are substituted into the algebraic equations of the control volumes next to the boundaries (algebraic absorption of the boundary condition into the nearest interior nodal equation). Two types of boundary conditions are used in this work: Dirichlet and Neumann. A detailed description of formulation and implementation of these boundary conditions is presented for a general variable

$\Phi = U, V, T, W$ in this section. The pressure at the boundary nodes is calculated by performing linear extrapolation of the pressure of interior nodes toward the boundaries. The extrapolation relations for pressures on the boundaries are subsequently used in all algebraic equations with implicit pressure terms.

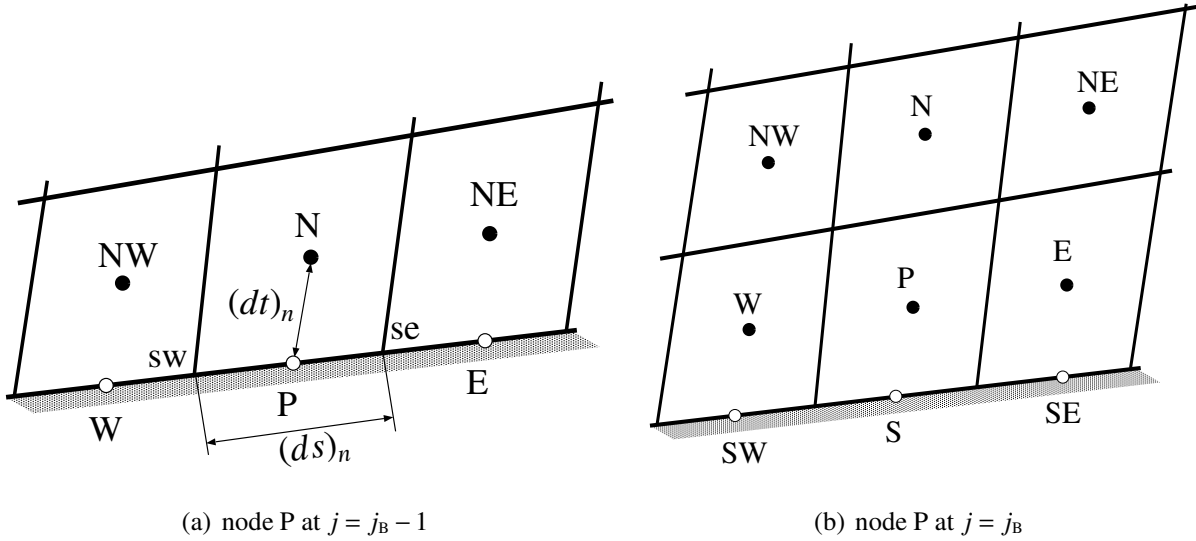


Figure 4.3: South boundary computational molecule.

The south boundary is used to illustrate the formulation of boundary conditions. Figure 4.3(a) shows a typical boundary node and its neighbours on the south boundary of the solution domain ($i, j = j_B - 1$). The algebraic equation that connects boundary node P to its adjacent internal node is as:

$$a_{P(i,j_B-1)}^{\phi,\phi} \Phi_{P(i,j_B-1)} + a_{N(i,j_B-1)}^{\phi,\phi} \Phi_{N(i,j_B-1)} = b_{(i,j_B-1)}^{\phi} \quad (4.119)$$

The coefficients of Equation (4.119) are set to the desired boundary conditions at the south boundary. The setting of these coefficients for the two boundary condition types is given below.

4.3.3.1 Dirichlet

This boundary condition is prescribed when the value of the variable Φ at the boundary is given. For Dirichlet boundary condition, the coefficients of Equation (4.119) are set to:

$$\begin{aligned} a_{P(i,j_B-1)}^{\phi,\phi} &= 1 \\ a_{N(i,j_B-1)}^{\phi,\phi} &= 0 \\ b_{(i,j_B-1)}^{\phi} &= \Phi_{\text{bnd}} \end{aligned} \quad (4.120)$$

where Φ_{bnd} is the Φ value at boundary.

4.3.3.2 Neumann

A Neumann boundary condition is applied when the gradient of a variable is prescribed at the boundary (e.g. $\frac{\partial \Phi}{\partial x} = \Gamma_{\text{bnd}}^{\phi}$). In the case of a non-orthogonal grid, $\frac{\partial \Phi}{\partial x}$ and $\frac{\partial \Phi}{\partial y}$ are specified in terms of the gradients along the unit vector directions, $\hat{s}$ and $\hat{t}$. The gradients along the west to east direction, $\hat{s}$, and south to north direction, $\hat{t}$, can be expressed in a chain rule as follows:

$$\frac{\partial \Phi}{\partial s} = \frac{\partial \Phi}{\partial x} \frac{\partial x}{\partial s} + \frac{\partial \Phi}{\partial y} \frac{\partial y}{\partial s} \quad (4.121)$$

$$\frac{\partial \Phi}{\partial t} = \frac{\partial \Phi}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial \Phi}{\partial y} \frac{\partial y}{\partial t} \quad (4.122)$$

The gradient of Φ in the x direction can be evaluated using Cramer's rule:

$$\frac{\partial \Phi}{\partial x} = \frac{\begin{vmatrix} \frac{\partial \Phi}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial \Phi}{\partial t} & \frac{\partial y}{\partial t} \end{vmatrix}}{\begin{vmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} \end{vmatrix}} = \frac{\frac{\partial \Phi}{\partial s} \frac{\partial y}{\partial t} - \frac{\partial \Phi}{\partial t} \frac{\partial y}{\partial s}}{\frac{\partial x}{\partial s} \frac{\partial y}{\partial t} - \frac{\partial y}{\partial s} \frac{\partial x}{\partial t}} \quad (4.123)$$

The gradient at the east face of a control volume becomes:

$$\left. \frac{\partial \Phi}{\partial x} \right|_e = \frac{\left. \frac{\partial \Phi}{\partial s} \right|_e \left. \frac{\partial y}{\partial t} \right|_e - \left. \frac{\partial \Phi}{\partial t} \right|_e \left. \frac{\partial y}{\partial s} \right|_e}{\left. \frac{\partial x}{\partial s} \right|_e \left. \frac{\partial y}{\partial t} \right|_e - \left. \frac{\partial y}{\partial s} \right|_e \left. \frac{\partial x}{\partial t} \right|_e} = \frac{\left. \frac{\partial \Phi}{\partial s} \right|_e t_{ye} - \left. \frac{\partial \Phi}{\partial t} \right|_e s_{ye}}{s_{xe} t_{ye} - t_{xe} s_{ye}} \quad (4.124)$$

A similar approach to Equation (4.124) can be applied to the north face of a control volume:

$$\left. \frac{\partial \Phi}{\partial x} \right|_n = \frac{\left. \frac{\partial \Phi}{\partial s} \right|_n \left. \frac{\partial y}{\partial t} \right|_n - \left. \frac{\partial \Phi}{\partial t} \right|_n \left. \frac{\partial y}{\partial s} \right|_n}{\left. \frac{\partial x}{\partial s} \right|_n \left. \frac{\partial y}{\partial t} \right|_n - \left. \frac{\partial y}{\partial s} \right|_n \left. \frac{\partial x}{\partial t} \right|_n} = \frac{\left. \frac{\partial \Phi}{\partial s} \right|_n t_{yn} - \left. \frac{\partial \Phi}{\partial t} \right|_n s_{yn}}{s_{xn} t_{yn} - t_{xn} s_{yn}} \quad (4.125)$$

The change in Φ in the y direction can be evaluate as:

$$\frac{\partial \Phi}{\partial y} = \frac{\left| \begin{array}{cc} \frac{\partial x}{\partial s} & \frac{\partial \Phi}{\partial s} \\ \frac{\partial x}{\partial t} & \frac{\partial \Phi}{\partial t} \end{array} \right|}{\left| \begin{array}{cc} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} \end{array} \right|} = \frac{\frac{\partial \Phi}{\partial t} \frac{\partial x}{\partial s} - \frac{\partial \Phi}{\partial s} \frac{\partial x}{\partial t}}{\frac{\partial x}{\partial s} \frac{\partial y}{\partial t} - \frac{\partial y}{\partial s} \frac{\partial x}{\partial t}} \quad (4.126)$$

Equation (4.126) can be written for the east and north face of a control volume as:

$$\left. \frac{\partial \Phi}{\partial y} \right|_e = \frac{\left. \frac{\partial \Phi}{\partial t} \right|_e \left. \frac{\partial x}{\partial s} \right|_e - \left. \frac{\partial \Phi}{\partial s} \right|_e \left. \frac{\partial x}{\partial t} \right|_e}{\left. \frac{\partial x}{\partial s} \right|_e \left. \frac{\partial y}{\partial t} \right|_e - \left. \frac{\partial y}{\partial s} \right|_e \left. \frac{\partial x}{\partial t} \right|_e} = \frac{\left. \frac{\partial \Phi}{\partial t} \right|_e s_{xe} - \left. \frac{\partial \Phi}{\partial s} \right|_e t_{xe}}{s_{xe} t_{ye} - t_{xe} s_{ye}} \quad (4.127)$$

$$\left. \frac{\partial \Phi}{\partial y} \right|_n = \frac{\left. \frac{\partial \Phi}{\partial t} \right|_n \left. \frac{\partial x}{\partial s} \right|_n - \left. \frac{\partial \Phi}{\partial s} \right|_n \left. \frac{\partial x}{\partial t} \right|_n}{\left. \frac{\partial x}{\partial s} \right|_n \left. \frac{\partial y}{\partial t} \right|_n - \left. \frac{\partial y}{\partial s} \right|_n \left. \frac{\partial x}{\partial t} \right|_n} = \frac{\left. \frac{\partial \Phi}{\partial t} \right|_n s_{xn} - \left. \frac{\partial \Phi}{\partial s} \right|_n t_{xn}}{s_{xn} t_{yn} - t_{xn} s_{yn}} \quad (4.128)$$

To implement the Neumann boundary condition on the south boundary of the domain, $\frac{\partial \Phi}{\partial y}$ on the north face of the zero-width boundary control volume must be set. The derivatives in Equation (4.128) are evaluated using nodal and corner values of Φ :

$$\left. \frac{\partial \Phi}{\partial y} \right|_{n(i,j_B-1)} = \Gamma_{\text{bnd}}^\phi = \frac{\frac{\Phi_N - \Phi_P}{(dt)_n} s_{xn} - \frac{\Phi_{ne} - \Phi_{nw}}{(ds)_n} t_{xn}}{s_{xn} t_{yn} - t_{xn} s_{yn}} \quad (4.129)$$

Equation (4.129) can be rearranged into the form of a linear algebraic equation:

$$\Phi_P - \Phi_N = -(\Phi_{ne} - \Phi_{nw}) \frac{(dt)_n}{(ds)_n} \frac{t_{xn}}{s_{xn}} - \Gamma_{\text{bnd}}^\phi (dt)_n \frac{s_{xn} t_{yn} - t_{xn} s_{yn}}{s_{xn}} \quad (4.130)$$

The coefficients of Equation (4.130) are as follows:

$$\left. \begin{aligned} a_{P(i,j_B-1)}^{\phi,\phi} &= 1, & a_{N(i,j_B-1)}^{\phi,\phi} &= -1 \\ b_{(i,j_B-1)}^\phi &= -(\Phi_{ne} - \Phi_{nw}) \frac{(dt)_n}{(ds)_n} \frac{t_{xn}}{s_{xn}} - \Gamma_{\text{bnd}}^\phi (dt)_n \frac{s_{xn} t_{yn} - t_{xn} s_{yn}}{s_{xn}} \end{aligned} \right\} \quad (4.131)$$

The corner values in Equation (4.131) are determined by performing linear interpolation between the nearest boundary nodal values. Under the circumstances where the control volume is at the corner of the domain, i.g. (i_B, j_B) and both boundaries are Neumann type, then $\Phi_{se} = \Phi(i_B, j_B)$. If one of the boundaries has Dirichlet boundary condition, then $\Phi_{se} = \Phi_{\text{bnd}}$.

4.3.3.3 Algebraic Absorption of the Boundary Conditions

The boundary nodes can be eliminated from the solution fields by being substituted to the algebraic equations of the interior nodes adjacent to the boundaries. To illustrate the process, Equation (4.78) is rewritten for node P adjacent to the south boundary in Figure 4.3(b):

$$\begin{aligned} a_{P(i,j_B)}^{\phi,\phi} \Phi_{P(i,j_B)} + a_{E(i,j_B)}^{\phi,\phi} \Phi_{E(i,j_B)} + a_{W(i,j_B)}^{\phi,\phi} \Phi_{W(i,j_B)} + a_{N(i,j_B)}^{\phi,\phi} \Phi_{N(i,j_B)} + a_{S(i,j_B)}^{\phi,\phi} \Phi_{S(i,j_B)} \\ + a_{NE(i,j_B)}^{\phi,\phi} \Phi_{NE(i,j_B)} + a_{NW(i,j_B)}^{\phi,\phi} \Phi_{NW(i,j_B)} + a_{SE(i,j_B)}^{\phi,\phi} \Phi_{SE(i,j_B)} + a_{SW(i,j_B)}^{\phi,\phi} \Phi_{SW(i,j_B)} = b_{(i,j_B)}^\phi \end{aligned} \quad (4.132)$$

The nodes SW, S, and SE are located at the boundary and controlled by the boundary conditions. For these nodes, the algebraic boundary condition equation, Equation (4.119), can be rewritten as:

$$a_{P(i-1,j_B-1)}^\phi \Phi_{SW(i,j_B)} + a_{N(i-1,j_B-1)}^\phi \Phi_{W(i,j_B)} = b_{(i-1,j_B-1)}^\phi \quad (4.133)$$

$$a_{P(i,j_B-1)}^\phi \Phi_{S(i,j_B)} + a_{N(i,j_B-1)}^\phi \Phi_{P(i,j_B)} = b_{(i,j_B-1)}^\phi \quad (4.134)$$

$$a_{P(i+1,j_B-1)}^\phi \Phi_{SE(i,j_B)} + a_{N(i+1,j_B-1)}^\phi \Phi_{E(i,j_B)} = b_{(i+1,j_B-1)}^\phi \quad (4.135)$$

The boundary nodes Φ_{SW} , Φ_S , and Φ_{SE} in Equation (4.132) are replaced with Equations (4.133) to (4.135) in order to eliminate boundary nodes. This substitution results in the following equation:

$$\begin{aligned} \left(a_{P(i,j_B)}^{\phi,\phi}\right)^\oplus \Phi_{P(i,j_B)} + \left(a_{E(i,j_B)}^{\phi,\phi}\right)^\oplus \Phi_{E(i,j_B)} + \left(a_{W(i,j_B)}^{\phi,\phi}\right)^\oplus \Phi_{W(i,j_B)} + a_{N(i,j_B)}^{\phi,\phi} \Phi_{N(i,j_B)} \\ + a_{NE(i,j_B)}^{\phi,\phi} \Phi_{NE(i,j_B)} + a_{NW(i,j_B)}^{\phi,\phi} \Phi_{NW(i,j_B)} = \left(b_{(i,j_B)}^\phi\right)^\oplus \end{aligned} \quad (4.136)$$

The new coefficients of Equation (4.136) are:

$$\left. \begin{aligned} \left(a_{P(i,j_B)}^{\phi,\phi}\right)^\oplus &= a_{P(i,j_B)}^{\phi,\phi} - a_{S(i,j_B)}^{\phi,\phi} \frac{a_{N(i,j_B-1)}^{\phi,\phi}}{a_{P(i,j_B-1)}^{\phi,\phi}} \\ \left(a_{N(i,j_B)}^{\phi,\phi}\right)^\oplus &= a_{E(i,j_B)}^{\phi,\phi} - a_{SE(i,j_B)}^{\phi,\phi} \frac{a_{N(i+1,j_B-1)}^{\phi,\phi}}{a_{P(i+1,j_B-1)}^{\phi,\phi}} \\ \left(a_{S(i,j_B)}^{\phi,\phi}\right)^\oplus &= a_{W(i,j_B)}^{\phi,\phi} - a_{SW(i,j_B)}^{\phi,\phi} \frac{a_{N(i-1,j_B-1)}^{\phi,\phi}}{a_{P(i-1,j_B-1)}^{\phi,\phi}} \\ \left(b_{(i,j_B)}^\phi\right)^\oplus &= b_{(i,j_B)}^\phi - a_{S(i,j_B)}^{\phi,\phi} \frac{b_{(i,j_B-1)}^\phi}{a_{P(i,j_B-1)}^{\phi,\phi}} \\ &\quad - a_{SE(i,j_B)}^{\phi,\phi} \frac{b_{(i+1,j_B-1)}^\phi}{a_{P(i+1,j_B-1)}^{\phi,\phi}} - a_{SW(i,j_B)}^{\phi,\phi} \frac{b_{(i-1,j_B-1)}^\phi}{a_{P(i-1,j_B-1)}^{\phi,\phi}} \end{aligned} \right\} \quad (4.137)$$

After the modification of the interior node coefficients to implement the boundary conditions, $a_{SW(i,j_B)}^{\phi,\phi}$, $a_{S(i,j_B)}^{\phi,\phi}$, and $a_{SE(i,j_B)}^{\phi,\phi}$ are set to zero.

4.3.3.4 Face Velocity Boundary Conditions

The face velocity boundary conditions are derived using the nodal boundary conditions and implemented using the coefficients of the continuity equation. The south boundary is used as an

example to illustrate the derivation of the face velocity boundary condition. The continuity equation for node P in Figure 4.3(b), can also be applied on the south boundary as follows:

$$\begin{aligned} & \left(a_{e(i,j_B-1)}^{c,u} U_e + a_{e(i,j_B-1)}^{c,v} V_e \right) + \left(a_{w(i,j_B-1)}^{c,u} U_w + a_{w(i,j_B-1)}^{c,v} V_w \right) \\ & + \left(a_{n(i,j_B-1)}^{c,u} U_n + a_{n(i,j_B-1)}^{c,v} V_n \right) + \left(a_{s(i,j_B-1)}^{c,u} U_s + a_{s(i,j_B-1)}^{c,v} V_s \right) = b_{P(i,j_B-1)}^c \end{aligned} \quad (4.138)$$

One can use Equation (4.138) to produce separate equations for U_s and V_s :

$$\begin{aligned} U_s = \frac{-1}{a_{s(i,j_B-1)}^{c,u}} & \left[\left(a_{e(i,j_B-1)}^{c,u} U_e + a_{e(i,j_B-1)}^{c,v} V_e \right) + \left(a_{w(i,j_B-1)}^{c,u} U_w + a_{w(i,j_B-1)}^{c,v} V_w \right) \right. \\ & \left. + \left(a_{n(i,j_B-1)}^{c,u} U_n + a_{n(i,j_B-1)}^{c,v} V_n \right) + a_{s(i,j_B-1)}^{c,v} V_s - b_{P(i,j_B-1)}^c \right] \end{aligned} \quad (4.139)$$

$$\begin{aligned} V_s = \frac{-1}{a_{s(i,j_B-1)}^{c,v}} & \left[\left(a_{e(i,j_B-1)}^{c,u} U_e + a_{e(i,j_B-1)}^{c,v} V_e \right) + \left(a_{w(i,j_B-1)}^{c,u} U_w + a_{w(i,j_B-1)}^{c,v} V_w \right) \right. \\ & \left. + \left(a_{n(i,j_B-1)}^{c,u} U_n + a_{n(i,j_B-1)}^{c,v} V_n \right) + a_{s(i,j_B-1)}^{c,u} U_s - b_{P(i,j_B-1)}^c \right] \end{aligned} \quad (4.140)$$

The coefficients $a_{s(i,j_B-1)}^{c,u}$ and $a_{s(i,j_B-1)}^{c,v}$ are set to be -1 and moved to act as a source term in Equations (4.139) and (4.140), respectively:

$$\begin{aligned} U_s = & \left(a_{e(i,j_B-1)}^{c,u} U_e + a_{e(i,j_B-1)}^{c,v} V_e \right) + \left(a_{w(i,j_B-1)}^{c,u} U_w + a_{w(i,j_B-1)}^{c,v} V_w \right) \\ & + \left(a_{n(i,j_B-1)}^{c,u} U_n + a_{n(i,j_B-1)}^{c,v} V_n \right) + a_{s(i,j_B-1)}^{c,v} V_s + a_{s(i,j_B-1)}^{c,u} \end{aligned} \quad (4.141)$$

$$\begin{aligned} V_s = & \left(a_{e(i,j_B-1)}^{c,u} U_e + a_{e(i,j_B-1)}^{c,v} V_e \right) + \left(a_{w(i,j_B-1)}^{c,u} U_w + a_{w(i,j_B-1)}^{c,v} V_w \right) \\ & + \left(a_{n(i,j_B-1)}^{c,u} U_n + a_{n(i,j_B-1)}^{c,v} V_n \right) + a_{s(i,j_B-1)}^{c,u} U_s + a_{s(i,j_B-1)}^{c,v} \end{aligned} \quad (4.142)$$

Only south and north mass flow rates in control volume P are needed to set the south boundary condition and the U and V velocity boundary conditions are set independently. These two requirements change Equations (4.141) and (4.142) as follows:

$$U_s - a_{n(i,j_B-1)}^{c,u} U_n = a_{s(i,j_B-1)}^{c,u} \quad (4.143)$$

$$V_s - a_{n(i,j_B-1)}^{c,v} V_n = a_{s(i,j_B-1)}^{c,v} \quad (4.144)$$

To obtain the Dirichlet boundary condition for U and V on the south boundary, the coefficients of Equations (4.143) and (4.144) are set as:

$$\left. \begin{aligned} a_{n(i,j_B-1)}^{c,u} &= 0 \\ a_{s(i,j_B-1)}^{c,u} &= U_{\text{bnd}} \end{aligned} \right\} \quad (4.145)$$

$$\left. \begin{aligned} a_{n(i,j_B-1)}^{c,v} &= 0 \\ a_{s(i,j_B-1)}^{c,v} &= V_{\text{bnd}} \end{aligned} \right\} \quad (4.146)$$

To obtain the Neumann boundary condition for U and V on the south boundary, the $\frac{\partial \Phi}{\partial y}$ is approximated from face to face across the control volume P:

$$\left. \frac{\partial \Phi}{\partial y} \right|_{(i,j_B)} = \Gamma_{\text{bnd}}^\phi = \frac{\frac{\Phi_n - \Phi_s}{(dt)_P} s_{xs} - \frac{\Phi_{se} - \Phi_{sw}}{(ds)_s} t_{xP}}{s_{xs} t_{yP} - t_{xP} s_{ys}} \quad (4.147)$$

Rearranging Equation (4.147) for Φ_s leads to:

$$\Phi_s - \Phi_n = -(\Phi_{se} - \Phi_{sw}) \frac{(dt)_P t_{xP}}{(ds)_s s_{xs}} - \Gamma_{\text{bnd}}^\phi (dt)_P \frac{s_{xs} t_{yP} - t_{xP} s_{ys}}{s_{xs}} \quad (4.148)$$

The coefficients in Equations (4.143) and (4.144) for U and V Neumann boundary conditions respectively are defined as:

$$\left. \begin{aligned} a_{n(i,j_B-1)}^{c,u} &= 1 \\ a_{s(i,j_B-1)}^{c,u} &= -(\Phi_{se} - \Phi_{sw}) \frac{(dt)_P t_{xP}}{(ds)_s s_{xs}} - \Gamma_{\text{bnd}}^u (dt)_P \frac{s_{xs} t_{yP} - t_{xP} s_{ys}}{s_{xs}} \end{aligned} \right\} \quad (4.149)$$

$$\left. \begin{aligned} a_{n(i,j_B-1)}^{c,v} &= 1 \\ a_{s(i,j_B-1)}^{c,v} &= -(\Phi_{se} - \Phi_{sw}) \frac{(dt)_P t_{xP}}{(ds)_s s_{xs}} - \Gamma_{\text{bnd}}^v (dt)_P \frac{s_{xs} t_{yP} - t_{xP} s_{ys}}{s_{xs}} \end{aligned} \right\} \quad (4.150)$$

The rest of the coefficients in Equation (4.138) are then set to zero.

To algebraically absorb the face boundary conditions into the interior nodal equations, Equations (4.143) and (4.144) are substituted to the continuity equation for node P:

$$\begin{aligned} & \left(a_{e(i,j_B)}^{c,u} U_e + a_{e(i,j_B)}^{c,v} V_e \right) + \left(a_{w(i,j_B)}^{c,u} U_w + a_{w(i,j_B)}^{c,v} V_w \right) + \left(a_{n(i,j_B)}^{c,u} U_n + a_{n(i,j_B)}^{c,v} V_n \right) \\ & + a_{s(i,j_B)}^{c,u} \left(a_{n(i,j_B-1)}^{c,u} U_n + a_{s(i,j_B-1)}^{c,u} \right) + a_{s(i,j_B)}^{c,v} \left(a_{n(i,j_B-1)}^{c,v} V_n + a_{s(i,j_B-1)}^{c,v} \right) = b_{P(i,j_B)}^c \end{aligned} \quad (4.151)$$

Collecting terms yields:

$$\left(a_{e(i,j_B)}^{c,u} U_e + a_{e(i,j_B)}^{c,v} V_e \right) + \left(a_{w(i,j_B)}^{c,u} U_w + a_{w(i,j_B)}^{c,v} V_w \right) + \left(\left(a_{n(i,j_B)}^{c,u} \right)^\oplus U_n + \left(a_{n(i,j_B)}^{c,v} \right)^\oplus V_n \right) = \left(b_{P(i,j_B)}^c \right)^\oplus \quad (4.152)$$

The new coefficients are then defined as:

$$\left. \begin{aligned} \left(a_{n(i,j_B)}^{c,u} \right)^\oplus &= a_{n(i,j_B)}^{c,u} + a_{s(i,j_B)}^{c,u} a_{n(i,j_B-1)}^{c,u} \\ \left(a_{n(i,j_B)}^{c,v} \right)^\oplus &= a_{n(i,j_B)}^{c,v} + a_{s(i,j_B)}^{c,v} a_{n(i,j_B-1)}^{c,v} \\ \left(b_{P(i,j_B)}^c \right)^\oplus &= b_{P(i,j_B)}^c - a_{s(i,j_B)}^{c,u} a_{s(i,j_B-1)}^{c,u} - a_{s(i,j_B)}^{c,v} a_{s(i,j_B-1)}^{c,v} \end{aligned} \right\} \quad (4.153)$$

4.3.4 E-factor

In development of the elliptic model in this work, the governing equations are made fully implicit. Although the steady-state solution is required in this study, the transient terms are used in the equations as relaxation in the solution of the coupled non-linear equations.

Van Doormaal and Raithby [102] recommended replacing the transient term with a distorted transient term. This distorted transient scheme uses a so-called E-factor, E . To use this scheme, $a_P^{u,u}$ equation, Equation (D.21), is rewritten as:

$$\left(a_P^{u,u} \right) = \frac{\rho_P \mathbf{V}_P}{\Delta t} + \left(a_P^{u,u} \right)^* \quad (4.154)$$

The transient term in Equation (D.21) is redefined using the E-factor:

$$\frac{\rho_P \mathbf{V}_P}{\Delta t} = \frac{\left(a_P^{u,u} \right)^*}{E^u} \quad (4.155)$$

Substituting Equation (4.155) into Equations (4.154) and (D.56) produces new definitions for $a_p^{u,u}$ and b_p^u coefficients:

$$(a_p^{u,u}) = (a_p^{u,u})^* + \frac{(a_p^{u,u})^*}{E^u} = \left(1 + \frac{1}{E^u}\right) (a_p^{u,u})^* \quad (4.156)$$

$$b_p^u = \frac{(a_p^{u,u})^*}{E^u} U_p^o + \rho_P g_x \nabla_P \quad (4.157)$$

A similar definition is used for the V , T , and ξ_W equations.

The E-factor allows taking a different Δt in each control volume (if control volumes have different sizes), which can lead to faster convergence. In the computer code implementation of the coefficient calculations, both the E-factor and true transient formulations are available and are selected through the specification of E and Δt values.

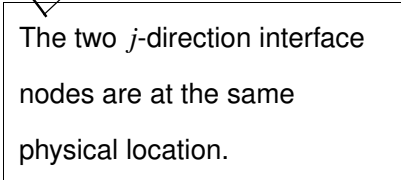
4.3.5 Interface Movement Procedure

The interface location is determined by imposing the mass balance at each column of the liquid region using the ILMB method. Equation (4.158) balances the mass crossing the east, west, and interface of the liquid column shaded in Figure 4.4.

$$\underbrace{\int_0^{h_{L,e}} \rho_{L,e} (\vec{V} \cdot \hat{n})_e dh}_{\dot{m}'_e} = \underbrace{\int_0^{h_{L,w}} \rho_{L,w} (\vec{V} \cdot \hat{n})_w dh}_{\dot{m}'_w} + \underbrace{\dot{m}'_{\text{intf}}}_{\text{mass crossing the interface}} \quad (4.158)$$

where $h_{L,w}$ and $h_{L,e}$ are the distance of the interface from the domain south boundary at the west and east side of the liquid column. The integrals in Equation (4.158) can be converted using a single integration point at each face of the control volumes.

$$\sum_{j=j_{BL}}^{j_{EL}} \rho_{L_e} (U_e n_{xe} + V_e n_{ye}) \Delta h_{L,e} = \sum_{j=j_{BL}}^{j_{EL}} \rho_{L_w} (U_w n_{xw} + V_w n_{yw}) \Delta h_{L,w} + \dot{m}'_{\text{intf}} \quad (4.159)$$



$$\frac{1}{N_{y,L}} \left[\sum_{j=j_{BL}}^{j_{EL}} \rho_{L_e} (U_e n_{xe} + V_e n_{ye}) \right] h_{L,e} = \frac{1}{N_{y,L}} \left[\sum_{j=j_{BL}}^{j_{EL}} \rho_{L_w} (U_w n_{xw} + V_w n_{yw}) \right] h_{L,w} + \dot{m}'_{\text{intf}} \quad (4.160)$$

gives the position of the interface at the successive stations along the domain south boundary.

4.3.6 Solution Method

Applying a finite volume method with the described techniques results in implicitly coupled algebraic equations. Using the non-orthogonal grid produces a nine-point computational molecule, consisting of the central node and its eight neighbouring nodes, for each field variable (U , V , P , T , and W in both phases). Therefore, the coefficients for each node are stored in a nine-banded 5-block matrix. Then all the coefficients are assembled in a sparse matrix. The interface condition coefficients are also added to the sparse matrix. An in-house computer code implements this numerical solution approach. The coupled algebraic equations are all solved together simultaneously using the parallelized SuperLU-DIST [103] direct solver within the PETSc software library.

4.3.6.1 Convergence Criteria

The numerical solution of the algebraic equations is repeated until a converged solution is obtained for the field variables and the interface movement. At each iteration the matrix equation is solved on a fixed mesh. Before repeating the numerical solution, the interface is moved based on the most recent interface height calculations and the entire domain grid is recalculated. The next iteration of the numerical solution begins with updating the coefficient matrix based on the most recent field variables and domain grid. The computation proceeds until the desired convergence is obtained.

The steady-state convergence of the field variables is checked using the following:

$$\left| \frac{\Phi_{(i,j)}^n - \Phi_{(i,j)}^{n-1}}{\max(\Phi_{\text{all}(i,j)}^n) - \min(\Phi_{\text{all}(i,j)}^n)} \right| \leq \epsilon^\phi \quad (4.161)$$

where ϵ^ϕ is the steady-state convergence criterion for the field variable Φ and n is the iteration number. In this study, $\epsilon^U = \epsilon^V = \epsilon^P = \epsilon^W = 10^{-7}$ and $\epsilon^T = 10^{-4}$. Convergence of the interface

height is declared when the maximum of all absolute changes in interface node locations between two consecutive iterations is less than 10^{-10} m for the entire domain.

The residual of the linearised governing equations are also monitored during the computation process using the following equation:

$$\{\mathcal{R}^n\} = |\{b\} - [A] \cdot \{\Phi^n\}| \leq \mathcal{R}_{\text{spec}}^\phi \quad (4.162)$$

where $\mathcal{R}^n$ is the absolute residual of variable Φ algebraic equation and $\mathcal{R}_{\text{spec}}^\phi$ is the specified residual criterion for each field variable. For a typical case in this study, $\mathcal{R}_{\text{spec}}^U = \mathcal{R}_{\text{spec}}^V = \mathcal{R}_{\text{spec}}^P = \mathcal{R}_{\text{spec}}^{\xi_w} = 10^{-6}$ and $\mathcal{R}_{\text{spec}}^T = 10^{-4}$. The time step size was adjusted for the simulations of the elliptic model. No change in the converged solution was observed with variation of the time step size.

Chapter 5

Evaporation Process inside Parallel-Plate Channels: Parabolic Model

5.1 Introduction

The results of the parabolic numerical model for the simulation of pure water liquid film in the vicinity of an gas-vapour stream in a parallel plate channel are presented in this chapter. Domain definition and boundary conditions for two-phase evaporation in a vertical channel are shown in Figure 2.1. Detailed results are compared with the literature to demonstrate the validity of the present approach. In the area of numerical models of falling film evaporation in vertical parallel plate channels, the present work has a similar formulation to previous studies but differs in two important ways. First, the method of solution is significantly different from previous studies using the parabolic equation set. The present numerical model is believed to be the first evaporation application of a fully-coupled technique in which all the field variables, the film thickness, and the pressure gradient are solved simultaneously. This technique is based on the approach developed by Siow [95], and provides robust solution behaviour and fast convergence. A complete set of parabolic governing equations is solved that includes fundamental interface balances and variable properties. A dynamically moving mesh is used that matches the liquid-gas interface at every axial location. Second, the present work provides new, detailed results that examine the effects of changing key parameters such as the wall heat flux, the inlet relative humidity, inlet film Reynolds number, and the pressure. Two aspects of the work that have not been seen in previous studies are (1) a focus on the results near the channel inlet that examines a sharp decrease in interface heat and mass transfer and (2) the effects of pressure changes on the thermal and mass buoyancy forces. The effects of parameter changes on the overall effectiveness of the system are also examined.

5.2 Grid independence study

A grid independence study was conducted using a typical case studied in this work (Case W6 described in Section 5.4). The axial profiles for the interface velocity, temperature, and air mass fraction were compared for different meshes. The range of the number of nodes in these tests were as follows: $20 \leq N_{y,L} \leq 80$, $80 \leq N_{y,M} \leq 240$, and $800 \leq N_x \leq 3200$. Comparing with the finest grid ($N_{y,L} = 80$, $N_{y,M} = 240$, and $N_x = 3200$), a grid with $N_{y,L} = 40$, $N_{y,M} = 160$, and $N_x = 1600$ had the maximum percent differences of 0.10, 0.17, and 0.25 for the interface velocity, temperature, and air mass fraction, respectively. These differences are considered to be sufficiently small, so the above-mentioned grid was used for all the results presented in this work.

5.3 Comparisons with previous works

5.3.1 Definitions of comparison cases

In this section, the results of the present model are compared to three earlier works that studied evaporation of air-water and air-ethanol in vertical parallel plate channels. Due to the opposing buoyancy effects of water evaporation in experimental studies in the literature and the limitation of the parabolic model for simulating the upward flows, air-water cases are only compared with the numerical works [9, 29]. For ethanol, the present numerical results are compared with previous experimental results [1] and numerical results [9]. Table 5.1 summarizes the operating parameters of the comparison cases.

In order to compare the results to those presented by Yan [9], the local Nusselt number and Sherwood number are respectively defined as follows:

$$\text{Nu}_{\text{intf}} = \frac{q''_{\text{intf}} (4H)}{k_M (T_{\text{intf}} - T_b)} \quad (5.1)$$

$$\text{Sh}_{\text{intf}} = \frac{\dot{m}''_{\text{intf}} W_{\text{intf}} (4H)}{\rho_M D^{AB} (W_b - W_{a,\text{intf}})} \quad (5.2)$$

Table 5.1: Definitions of comparison cases

Case	Authors	Method ^a	Re _{M,in}	Fr _{L,in}	$\dot{m}'_{L,in}$ [kg/(m·s)]	T _{L,in} [°C]	T _{M,in} [°C]	q'' _{wall} [W/m ²]
W1-a	Yan [9]	N	2000	3.34	0.04	20	20	500
W1-b								1000
W1-c								3000
W2	[29]	N	100	3.66	0.01	25	25	8000
E1-a	[1]	E	650	4.2	0.01	40	31.5	0
E1-b				8.4	0.02			
E1-c				16.8	0.04			
E2-a	[9]	N	2000	11.71	0.04	20	20	500
E2-b								1000
E2-c								3000

^aN represents Numerical and E represents Experimental

where the local bulk temperature T_b and local bulk mass fraction W_b are defined as:

$$T_b = \frac{\int_{\delta}^{2H} \rho_M C_{p,M} U_M T dy}{\int_{\delta}^{2H} \rho_M C_{p,M} U_M dy} \quad (5.3)$$

$$W_b = \frac{\int_{\delta}^{2H} \rho_M U_M W dy}{\int_{\delta}^{2H} \rho_M U_M dy} \quad (5.4)$$

Figure 5.1 compares the results of the present work with Yan [9] for Case W1. The results for heat and mass transfer of the present work and those of Yan have very similar trends. The maximum percent differences between the present study and Case W1 are 8.4 and 4.5 for Nu_{intf} and Sh_{intf} , respectively. These deviations can be due to the differences in equations solved. In the

Yan [9] analysis for Case W1, the inertial term in the momentum equation for the liquid phase has been neglected. In addition, different mass balance and pressure gradient calculations have been used by Yan [9]. Differences in the calculation of thermophysical properties could also contribute to the deviations.

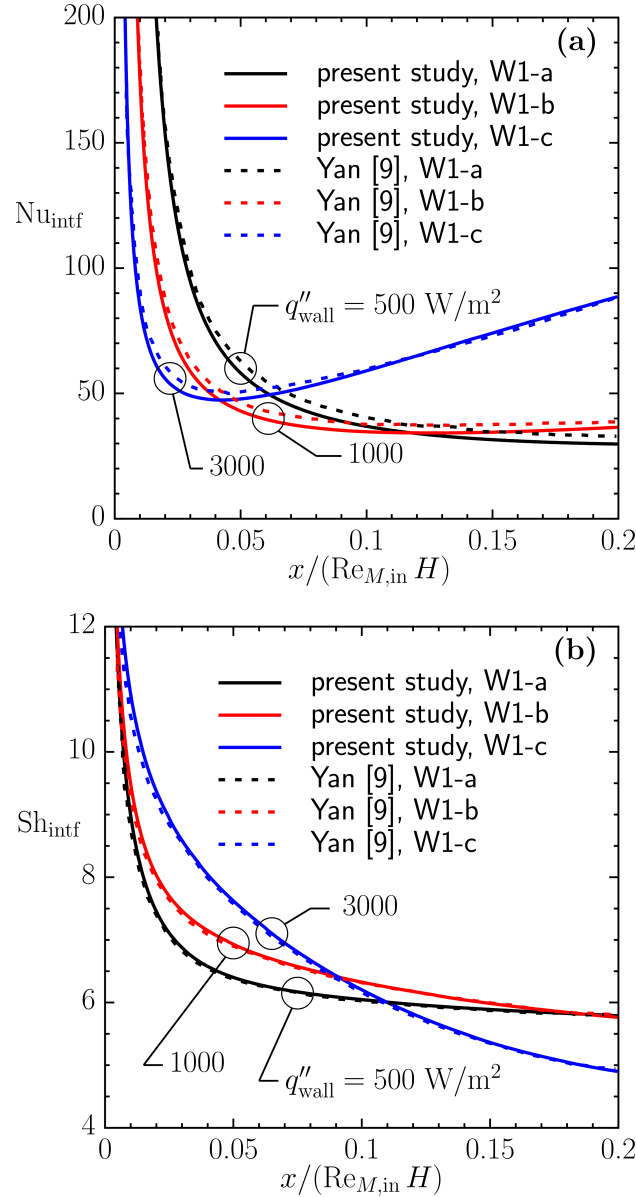


Figure 5.1: Comparison of axial variation of interface (a) Nu number and (b) Sh number, for Case W1

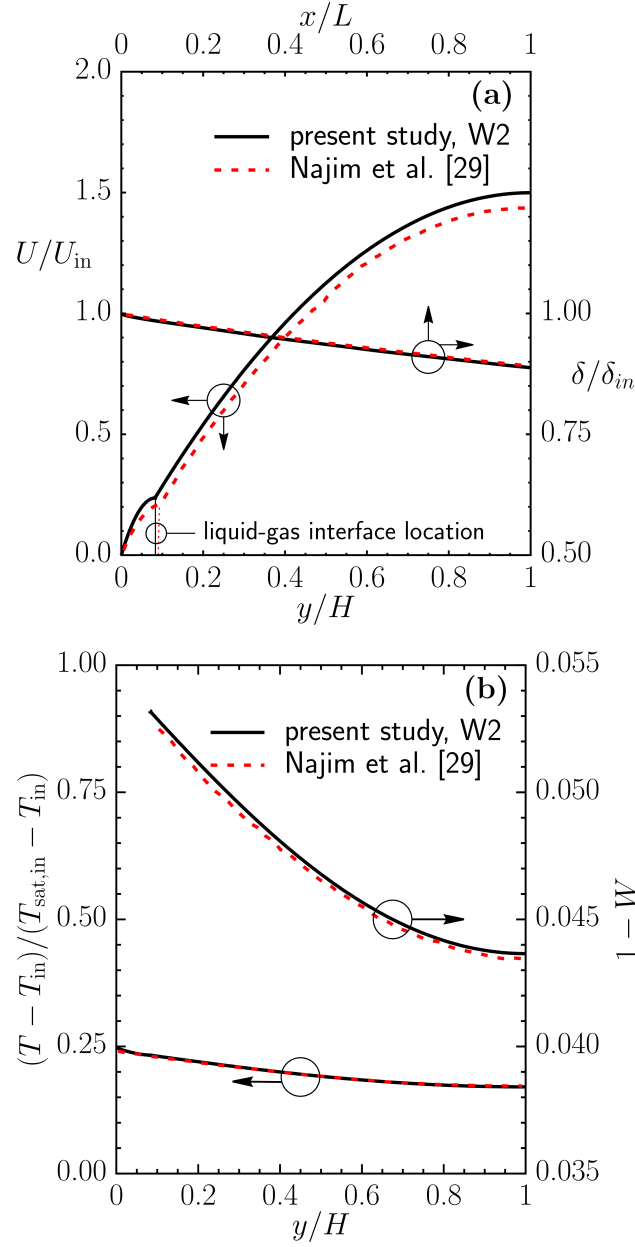


Figure 5.2: Comparison of (a) velocity and film thickness and (b) temperature and vapour mass fraction for Case W2

Figure 5.2 compares the results of the present study to Najim et al. [29] for Case W2. The comparison has been done for the film thickness and for the velocity, temperature, and vapour

mass fraction in transverse direction at the channel exit. The trends of the results are similar, but there are small differences between the results which are expected to be due to some differences in the procedures for calculating the film thickness and pressure gradient. The maximum percent differences between the current work and Najim et al. [29] are 21.1, 1.6, 0.12, and 0.9 for velocity, film thickness, temperature, and vapour mass fraction, respectively.

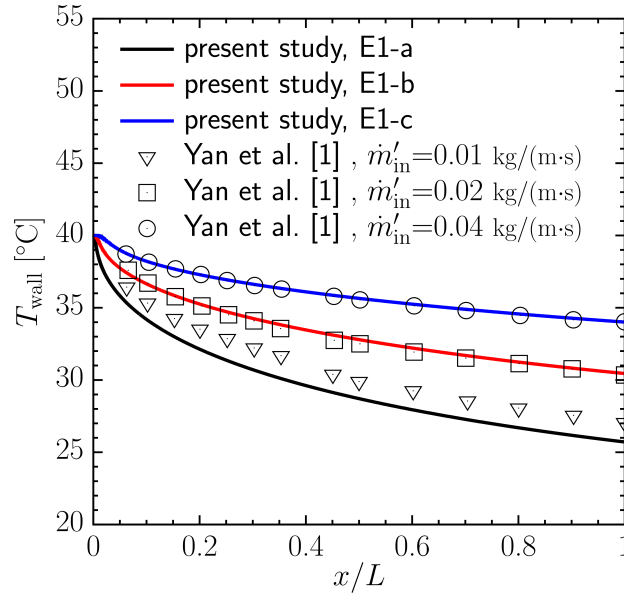


Figure 5.3: Comparison of temperature distribution at the wall for Case E1

The case of ethanol evaporation is compared with Yan et al. [1] for Case E1 in Figure 5.3. The results are in good agreement with experimental measurements. The highest deviation is for the lowest liquid mass flow rate with a maximum percent difference of 5.6. The difference can be due to the presence of ethanol vapour at the inlet, which was inevitable in the experimental study as mentioned by Yan and Lin [104].

The present results were also compared to Yan [9] for Case E2. Initially, there were some differences between the results obtained by the present model and Yan for Case E2. It has been determined that these differences were due to a simplification of the spatial variation of $C_{p,L}$ made in the previous work [9]. In the previous study, the specific heat of the liquid film, $C_{p,L}$, did not change with temperature in axial and transverse directions inside a control volume and was

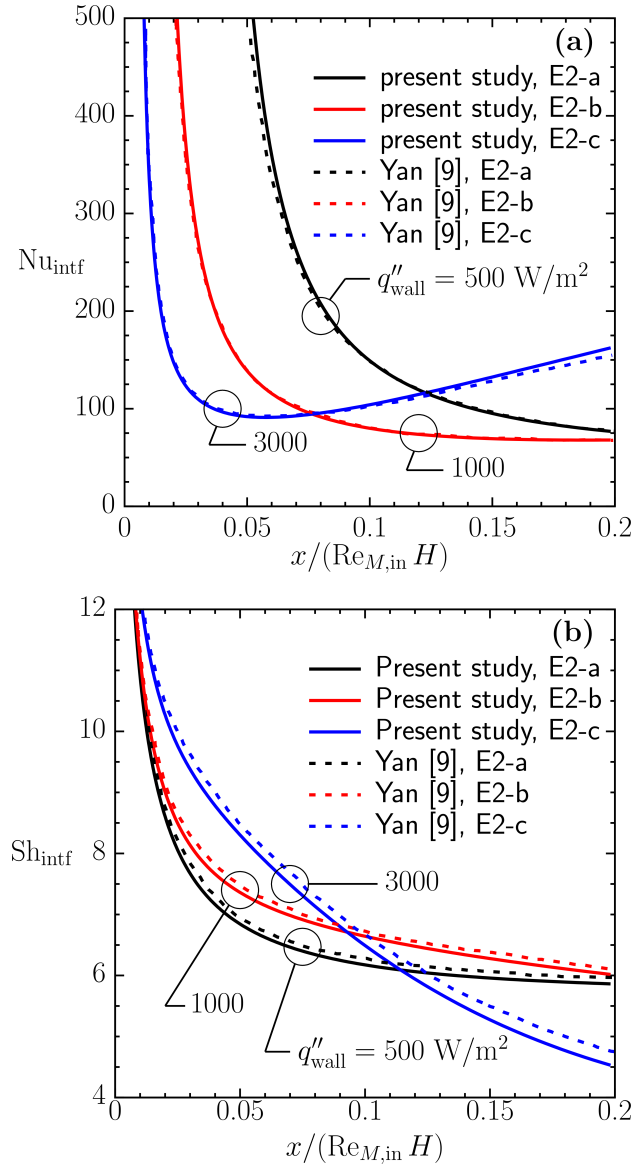


Figure 5.4: Comparison of axial variation of interface (a) Nu number and (b) Sh number for Case E2

determined by the temperature nodal value. Therefore, the gradients $\frac{\partial C_{p,L}}{\partial y}$ and $\frac{\partial C_{p,L}}{\partial x}$ were ignored in the advection terms of the liquid energy equation. This simplification is reasonable only when the change of specific heat with temperature is not significant. In Case E2, it was found that assuming a constant specific heat at the faces of each control volume resulted in an under-prediction of the

advected energy. In the present model, the liquid specific heat changes with temperature in the energy equation, and an upwind scheme is applied at the east face and the west face, so the liquid specific heat is different at the east and west faces of every control volume. It is important to note that this issue does not occur for Case W1 because the liquid specific heat of water changes by less than 0.05% for the temperature range of 290 to 350 K. However, for ethanol, the liquid specific heat increases by about 33% with increasing temperature over the same temperature range, which has been shown in Fig. 5 in [29]. For comparison purposes, the present model was temporarily modified to keep the liquid specific heat constant on east and west faces. Figure 5.4 shows the good agreement obtained using this approach. The maximum percent differences in Nu and Sh are 7.7% and 4.9%, respectively, for the highest wall heat flux case. The slight differences between the current results and Case E2 are expected to be due to the reasons mentioned for Case W1.

The good agreement with previous numerical and experimental studies in this area demonstrates the accuracy and reliability of the present model. The model will now be used for detailed exploration of aspects of falling film evaporation in vertical channels that were not addressed in earlier works.

5.4 Results and discussion

5.4.1 Parametric study discussion

In order to study the effects of operating parameters on the evaporation process, the co-current developing flow of liquid and mixture is modelled using the full original model discussed earlier. For given film and gas Reynolds numbers, the equations presented in Appendix A are utilized to specify the inlet liquid and mixture velocity fully-developed profiles along with the corresponding film thickness and pressure gradient. The common input parameters for all simulations in this section are: $L = 2$ m, $H = 0.015$ m, $T_{L,in} = 20^\circ\text{C}$, $T_{M,in} = 20^\circ\text{C}$, and $\text{Re}_{M,in} = 2000$. The wall heat flux changes from 500 to 4000 Wm^{-2} . The inlet liquid Reynolds number varies between 50 and

200. The range of inlet pressure is from 1 to 3 atm. The air mass fraction is calculated using the mixture relative humidity based on the method presented by Hassaninejadfarahani et al. [96]. For water, the relative humidity changes from 20% to 80%. For ethanol, the relative humidity is always zero at the inlet. The analysis of ethanol evaporation into air neglects the occurrence of water in the air and water absorption into the ethanol.

Tables 5.2 and 5.3 indicate the operating parameters for parametric study cases for water and ethanol, respectively. Some water cases will be used to study the effects of wall heat flux and inlet

Table 5.2: Parametric study cases for water

Case	$Re_{L,in}$	$Fr_{L,in}$	P [atm]	ϕ_{in} (%)	q''_{wall} [W/m ²]	$\overline{Gr}_T$	$\overline{Gr}_M$	$Gr_Q(\times 10^{-4})$
W3	50	4.18	1	50	500	24.4	9.9	14.6
W4	50	4.18	1	50	1000	51.2	18.7	29.2
W5	50	4.18	1	50	2000	97.1	46.7	58.4
W6	50	4.18	1	50	4000	162.4	136.5	116.9
W7	100	8.36	1	50	1000	29.3	11.3	29.2
W8	100	8.36	1	20	1000	27.7	13.7	29.1
W9	100	8.36	1	80	1000	31.0	8.8	29.4
W10	100	8.32	2	50	1000	127.3	23.7	116.4
W11	100	8.31	3	50	1000	294.6	36.3	261.6

relative humidity changes in Section 5.4.2 and details of the flow near the inlet in Section 5.4.3. Ethanol cases will be used for comparison with water cases to illustrate the effects of buoyancy forces and the effects of pressure change in Section 5.4.4. The Grashof numbers mentioned in Tables 5.2 and 5.3 will be discussed in Section 5.4.4.

Table 5.3: Parametric study cases for ethanol

Case	$Re_{L,in}$	$Fr_{L,in}$	P [atm]	q''_{wall} [W/m ²]	$\overline{Gr}_T$	$\overline{Gr}_M$	$Gr_Q(\times 10^{-4})$
E3	50	4.21	1	1000	32.2	-60.1	29.0
E4	50	4.21	1	2000	67.8	-101.4	58.0
E5	50	4.21	1	4000	117.0	-184.9	116.0
E6	100	8.34	1	1000	18.0	-48.0	29.0
E7	100	8.32	2	1000	89.0	-105.2	116.0
E8	100	8.30	3	1000	213.8	-163.1	260.9

5.4.2 Effects of wall heat flux and relative humidity change

Figure 5.5 presents the effects of changing the wall heat flux on the interfacial heat and mass transfer for cases W3 to W6. For Case W6, the supersaturation occurs after $x/L = 0.51$ due to the high amount of evaporated vapor added to the mixture, so the data after this location has been eliminated. As expected, the heat and mass transfer at the interface increase with increased wall heat flux. A higher wall heat flux adds more energy as sensible heat to the liquid, increasing the interfacial temperature. As a result, more energy and mass are transferred to the gas phase and the evaporation rate increases along the channel. By increasing the wall heat flux, the minimum in the interfacial heat transfer moves towards the channel inlet. Higher wall heat flux significantly affects the evaporation rate, even in the region near the inlet.

A better understanding of the heat and mass transfer process is obtained by examining the total evaporation mass flow rate per unit depth up to a given x location:

$$\dot{m}'_{\text{intf,tot}}(x) = \sum_{x_i=0}^x J'_{\text{intf}}(x_i) \quad (5.5)$$

Figure 5.6 shows the distribution of $\dot{m}'_{\text{intf,tot}}$ along the channel for different wall heat flux values. A higher evaporation rate is observed for higher wall heat flux. Increasing the wall heat flux

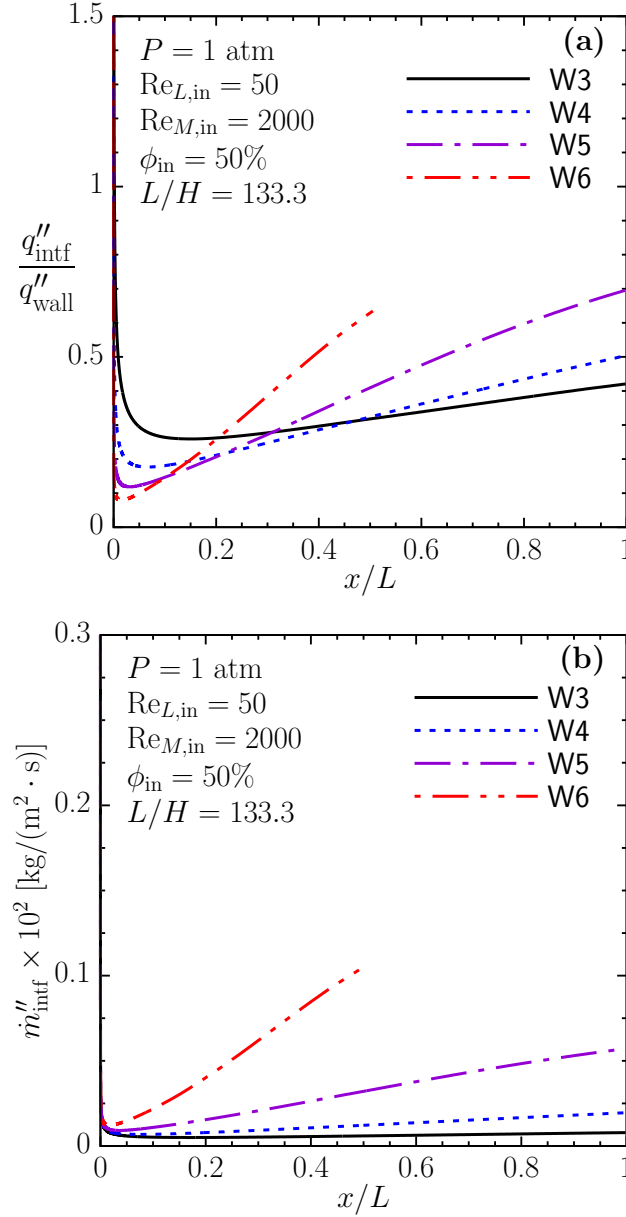


Figure 5.5: Axial variation of interfacial (a) heat flux and (b) mass flux, for different wall heat fluxes; $T_{L,\text{in}} = T_{M,\text{in}} = 20^\circ\text{C}$

adds more energy to the system as sensible and latent heat. The liquid falling film absorbs the energy received from the wall. Part of this energy is consumed to increase the liquid and mixture temperature. The rest of the energy added to the system leads to an increase in the evaporation rate.

The total evaporation mass flow rate for the entire channel increases more than two times when the wall heat flux increases from 1000 to 2000 [W/m²].

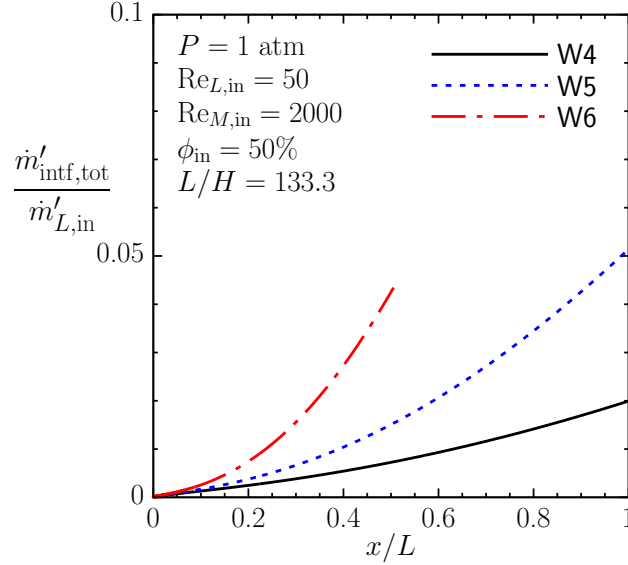


Figure 5.6: Axial variation of total evaporation mass flow rate per unit depth for different wall heat fluxes

Figure 5.7 shows the change of film thickness along the channel length. As the evaporation process occurs, mass of film is transferred to the mixture stream. The more heat added to the system, the more liquid is transferred to the gas phase through the latent heat transfer process, thereby decreasing the film thickness.

Three cases with $\phi_{\text{in}} = 20\%$, 50% , and 80% have been studied to investigate the effects of mixture relative humidity on the evaporation rate. As seen in Figure 5.8a, the interfacial heat flux is higher for a lower relative humidity. The mass flux changes the amount of energy transfer at the interface. Therefore, even though the amount of energy enter is the same, the energy transfer at the interface is different due to the different mass flux at the interface. A higher amount of air in the mixture leads to a more considerable concentration difference between the interface and gas phase. A decrease in the relative humidity causes an increase in the mass fraction gradient increases at the interface and a higher evaporation rate, as seen in Figure 5.8b.

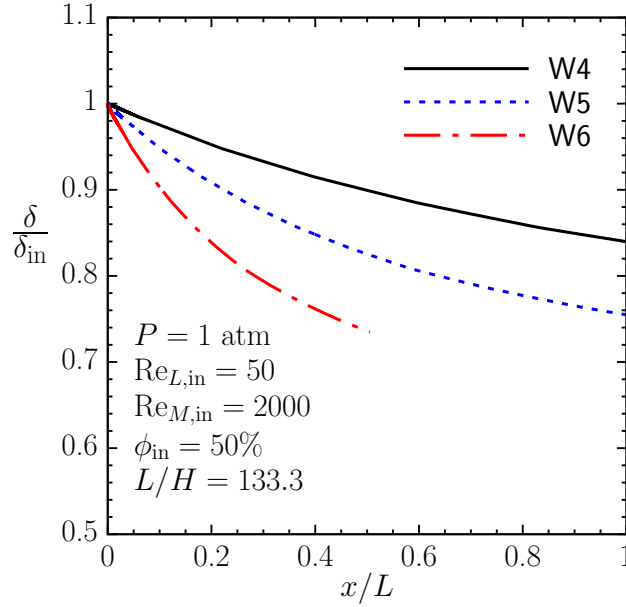


Figure 5.7: Axial variation of film thickness for different wall heat fluxes

5.4.3 Detail of the flow near the inlet

It was seen in Figure 5.5 that there is a substantial decrease in heat and mass transfer which occurs near the inlet. Near the inlet, the interfacial heat transfer is higher than the wall heat flux, as seen in Figure 5.5a. This trend revealed an interesting process that is responsible for the evaporation in that region and its sudden decrease. Case W3 was selected to study parameters affecting the heat and mass transfer in the inlet region. To determine the factors leading to the decrease of q''_{intf} near the inlet, transverse distributions of the vapour mass fraction and temperature in this region and farther along the channel were examined. Figure 5.9a shows the vapour mass fraction at selected axial locations near the inlet. The profiles are all equal and constant for $1.4 \leq \eta \leq 2$ near the inlet, so this range is not shown in the figure. There is a significant increase of the vapour mass fraction near the interface because of the concentration difference between the interface and the mixture. That difference leads to the mass diffusion of water vapour into the gas near the inlet. As also observed by Tsay et al. [15], the mass transfer process absorbs a substantial amount of energy as the latent heat for the vaporization of the liquid film. The latent heat transfer to the mixture is always

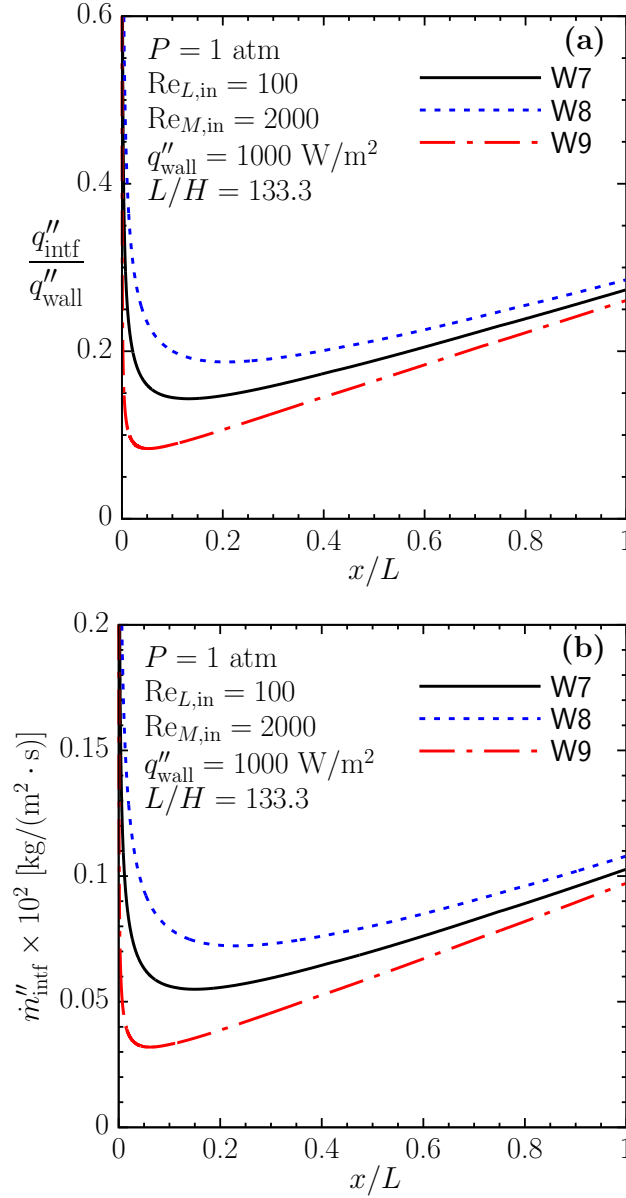


Figure 5.8: Axial variation of interfacial (a) heat flux and (b) mass flux, for different inlet relative humidities

positive, showing that evaporation always occurs instead of condensation. Note that the diffusion of vapour into the mixture region reduces the vapour mass fraction gradient at the interface; for instance, the vapour mass fraction gradient decreases about ten times from the region very close

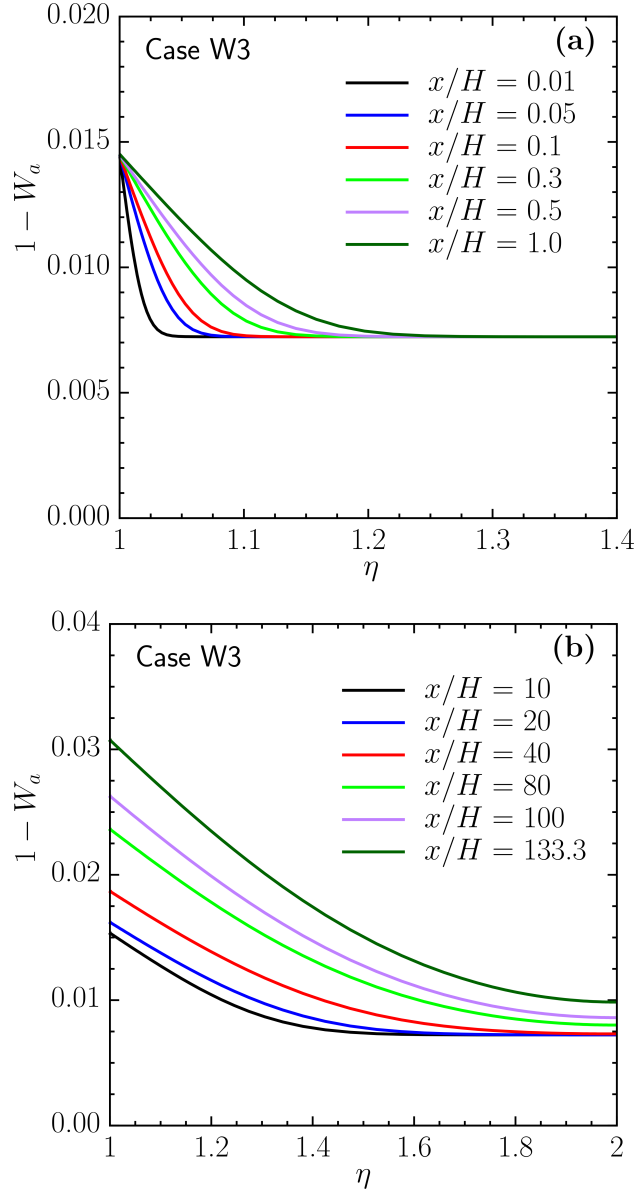


Figure 5.9: Vapour mass fraction at selected axial locations (a) near the inlet and (b) farther along the channel

to the inlet to $x/H = 0.5$. The increase of water vapour near the interface, and the subsequent decrease in the water vapour mass fraction gradient leads to a sharp decrease of evaporation rate along the channel length up to $x/H = 1$. Figure 5.9b shows mass fraction distribution at different

axial locations farther along the channel. As seen in this figure, the vapour mass fraction increases in the transverse direction due to the diffusion of vapour into the mixture phase. There is a slight increase in the vapour mass fraction gradient along x direction because the interfacial heat flux increases gradually.

Figure 5.10 shows the temperature distributions in liquid and mixture regions at selected axial locations. The liquid and mixture enter the channel at equal temperature (293.15 K). Just downstream of the inlet, the wall temperature increases slightly due to the heat flux at the wall, as seen in Figure 5.10a. At the interface, however, the temperature distribution is quite different. The direction of heat transfer in the liquid is from the liquid to the interface which corresponds to latent heat removal due to the mass flux at the interface. For the gas, however, the sensible heat transfer is from the gas to the interface. As a result, both liquid and gas lose some energy through the sensible heat transfer, causing a temperature decrease in both phases. This interfacial temperature reduction, however, is small in magnitude. So, it can be concluded that the temperature reduction does not affect the evaporation process significantly, and the decrease of mass fraction gradient plays the most important role in the sudden decline of the evaporation rate near the channel inlet. As seen in Figure 5.10b, farther along the channel, the temperature of the liquid and mixture increases due to the wall heat added, and the direction of mixture sensible heat transfer is from the interface to the mixture.

5.4.4 Effects of buoyancy forces and pressure change

There are two types of buoyancy forces in this system: thermal and solutal. The thermal buoyancy force always acts upwards and opposes the flow when energy is added to the gas phase and the interfacial temperature is higher than the mixture temperature. Depending on the molecular weight of the liquid relative to the air, the solutal buoyancy force can act either upwards or downwards. If the molecular weight of the liquid is less than the air, the solutal buoyancy acts upwards (opposing); otherwise, it acts downwards (aiding). As measures of the thermal and solutal buoyancy forces,

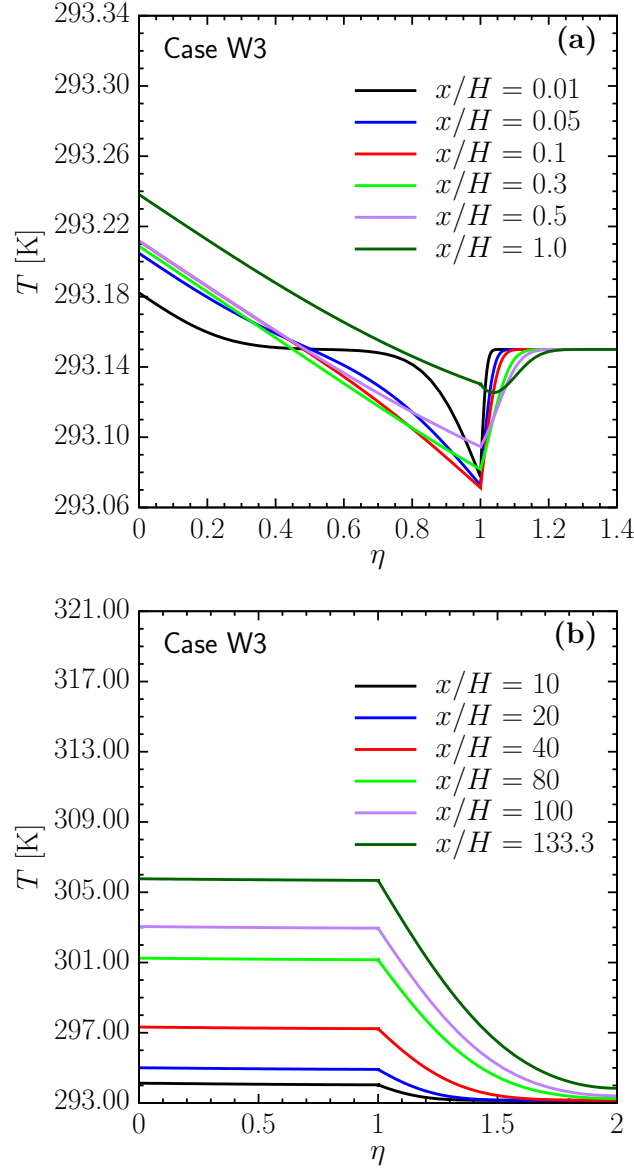


Figure 5.10: Temperature distribution at selected axial locations (a) near the inlet and (b) farther along the channel

Yan et al. [105] defined Grashof numbers based on the wall temperature and saturated mass fraction of vapour at the wall temperature and the inlet pressure. In this study, however, local Grashof

numbers are defined based on the interface temperature and mass fraction:

$$\text{Gr}_T = \frac{g (T_{\text{intf}} - T_{M,\text{in}}) H^4}{L v_M^2 T_{M,\text{in}}} \quad (5.6)$$

$$\text{Gr}_M = \frac{g (M_a/M_v - 1) (W_{a,\text{in}} - W_{a,\text{intf}}) H^4}{L v_M^2} \quad (5.7)$$

The axial variations of the thermal and mass Grashof numbers for Case W4 are shown in Figure 5.11. Towards the end of the channel, the local Grashof numbers are always increasing. Trends

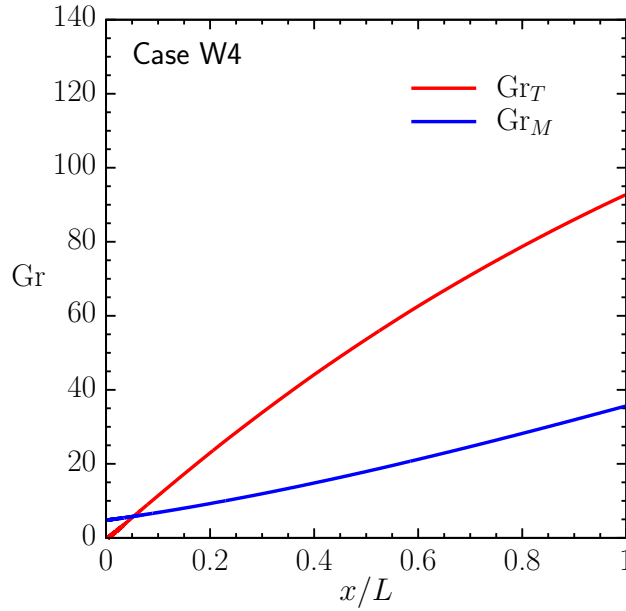


Figure 5.11: Axial variation of local Grashof numbers

in Figure 5.11 are similar across all cases examined in this study.

Average Grashof numbers can be defined as:

$$\overline{\text{Gr}}_T = \frac{1}{L} \int_0^L \text{Gr}_T dx \quad (5.8)$$

$$\overline{\text{Gr}}_M = \frac{1}{L} \int_0^L \text{Gr}_M dx \quad (5.9)$$

A Grashof number can also be defined based on the wall heat flux, which remains constant along the channel.

$$\text{Gr}_Q = \frac{g \beta q''_{\text{wall}} H^4}{k_M v_M^2} \quad (5.10)$$

It is proposed that the buoyancy forces are aiding if the sum of the average thermal and mass Grashof numbers is negative, and the buoyancy forces are opposing if the sum of the average Grashof numbers is positive.

As indicated in Tables 5.2 and 5.3, the average thermal Grashof number is always positive for both substances. The average mass Grashof number is always negative for ethanol and positive for water, indicating the aiding and opposing effect of solutal buoyancy for ethanol and water, respectively. For water, the average Grashof numbers increase by increasing the wall heat flux, due to the higher evaporation rate. The higher evaporation rate increases the vapour mass fraction at the interface, increasing the mass Grashof number. An increased vapour mass fraction also affects the vapour partial pressure (Equation (2.12)), resulting in the increase of interfacial temperature and thermal Grashof number. For ethanol, the increase of wall heat flux increases both Grashof numbers, but the magnitude of the average thermal Grashof number never exceeds that of the average mass Grashof number. Therefore, regardless of the value of wall heat flux used in this study, the net effect of the buoyancy forces is always aiding for ethanol.

The effects of inlet pressure change on the average thermal and mass Grashof numbers is also presented in Tables 5.2 and 5.3. For the ethanol cases listed at atmospheric pressure, the effect of mass transfer buoyancy is always more substantial than thermal buoyancy. The increase of pressure affects both buoyancy forces due to the density change, but it is more significant for the thermal force. A pressure increase reduces the evaporation rate and the interfacial mass fraction of vapour in the mixture, so the thermal diffusion becomes more considerable than mass diffusion during the evaporation process, resulting in a stronger opposing force.

Figure 5.12 depicts the effects of pressure change on the velocity profile at the channel exit. For constant $Re_{M,in}$, the inlet gas velocity decreases when the inlet pressure increases. As indicated in this figure, the velocity decreases near the interface due to increased opposing buoyancy force at higher pressures. For both substances, the velocity profiles are in accordance with the trends in the average Grashof numbers. Figure 5.12b shows that for ethanol the velocity decrease near

the interface is only observed for the highest pressure where the average thermal Grashof number exceeds the average mass Grashof number, as presented in Table 5.3. For combinations of higher inlet pressure and wall heat flux, the interface velocity can become negative, which terminates the marching solution; an elliptic model would be needed to model the reverse flow.

The effect of inlet pressure change on the interfacial heat flux is presented in Figure 5.13. The heat transfer decreases along the channel by increasing the inlet pressure. With increased pressure, the combination of a higher saturation temperature and reduced mixture velocity (for fixed $Re_{M,in}$) leads to an evaporation rate reduction. As indicated in Figure 5.14, the total evaporation rate of ethanol at the channel exit is more than four times higher than that of water for all pressure values. This trend occurs because the ethanol film is more volatile than water film. When changing the pressure from 1 atm to 3 atm, the total evaporation mass flow rate decreases by 65.4% and 59.61% for water and ethanol, respectively, showing the effect of pressure change on the evaporation rate is similar for the two substances.

5.4.5 Effectiveness

Another possible means of evaluating cases is a comparison of the total evaporation mass flow rate to the mass flow rate that could be evaporated based on the per unit depth total wall heat transfer rate and latent heat of vaporization. In the present study, this ratio is referred to as the effectiveness, ε , and is defined as:

$$\varepsilon = \frac{\dot{m}'_{L,in} - \dot{m}'_{L,out}}{(q''_{wall} L)/h_{fg}} \times 100 \quad (5.11)$$

For calculation of ε , h_{fg} was evaluated at the channel inlet conditions. Figure 5.15a shows the effectiveness of a system with $q''_{wall} = 1000 \text{ [W/m}^2\text{]}$ and $P_{in} = 1 \text{ [atm]}$ at various inlet liquid Reynolds numbers. The effectiveness decreases by increasing the liquid inlet Reynolds number. A higher liquid mass flow rate increases the amount of energy needed for heating the liquid film, which results in lower interfacial temperature for the same wall heat flux. Also, the advected energy by the liquid along the channel increases for higher liquid flow rates, reducing the amount of latent heat

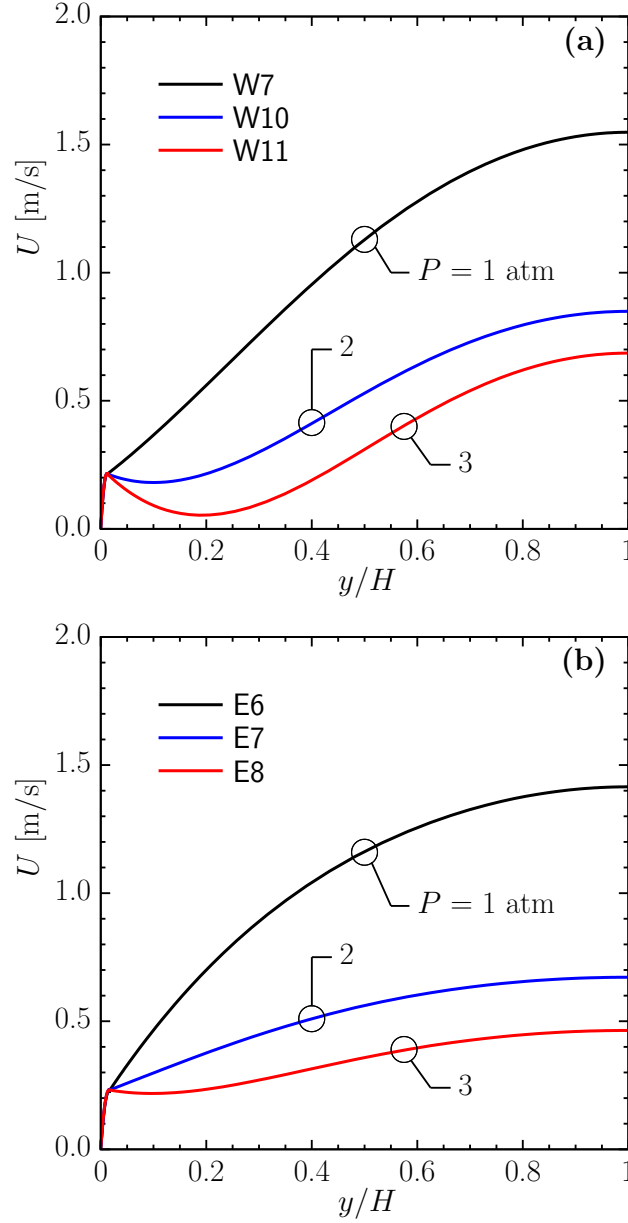


Figure 5.12: Velocity profile for different inlet pressure values at the channel exit for (a) selected water cases and (b) selected ethanol cases

transfer and the evaporation rate. The effectiveness of the system decreases 34.7% when changing $Re_{L,in}$ from 50 to 200 for ethanol. For water, the effectiveness decreases 60.2% when changing $Re_{L,in}$ over the same range. The effectiveness of ethanol cases is more significant than water due to

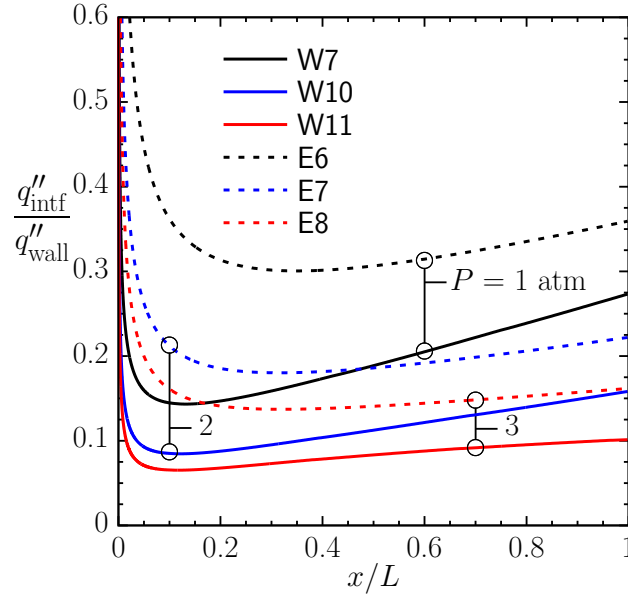


Figure 5.13: Axial variation of interfacial heat flux for different inlet pressures

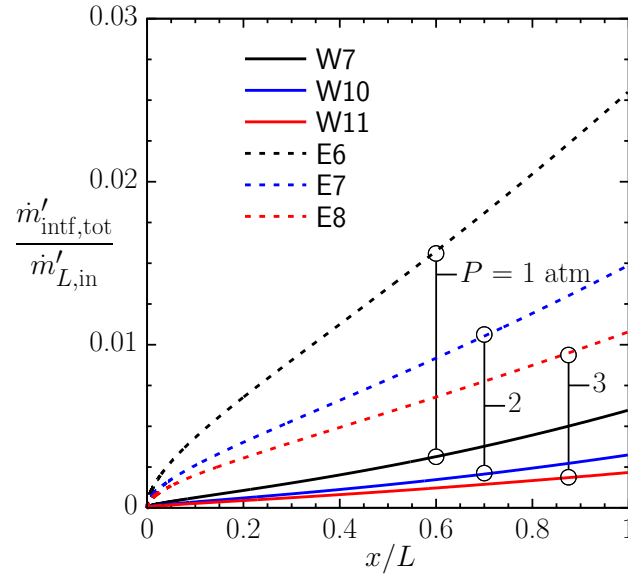


Figure 5.14: Axial variation of total evaporation mass flow rate per unit depth for different inlet pressures

the higher volatility of ethanol. Figure 5.15b shows the impact of inlet pressure on the effectiveness of a system with $q''_{\text{wall}} = 1000 \text{ [W/m}^2\text{]}$ and $\text{Re}_{L,\text{in}}=100$. The effectiveness decreases by increasing

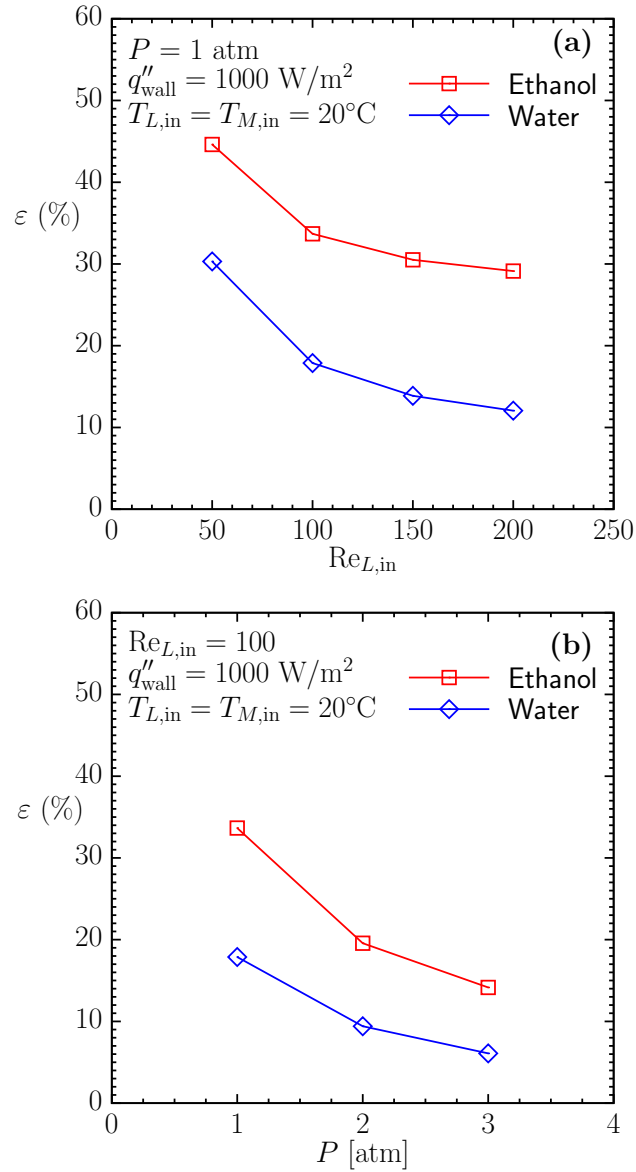


Figure 5.15: Effectiveness variation with (a) change in inlet liquid Reynolds number and (b) change in inlet pressure

the inlet pressure for both substances. From $P=1$ [atm] to 3 [atm], the effectiveness is reduced by 61.4% and 65.88% for ethanol and water, respectively.

Chapter 6

Evaporation Process inside Parallel-Plate Channels: Elliptic Model

6.1 Introduction

The results of the elliptic numerical model for the simulation of pure water liquid falling film inside a partially heated parallel plate channel are presented in this chapter. Reviewing the literature indicates that the numerical study of mixed convection of two-phase flows is mainly confined to the parabolic modelling results, so the effects of opposing buoyancy forces on the evaporation process have not been thoroughly investigated. In addition, none of the previous studies discussed the effect of the supersaturation phenomenon that may occur during the evaporation process. In this chapter, the effects of mixed convection and buoyancy forces on the flow and thermal characteristics of the evaporation process of liquid water falling film inside a vertical parallel plate channel are investigated. Moreover, a novel numerical method is proposed to address supersaturation in the system. The elliptic equation approach enables prediction of reverse flow. By contrast, an approach using parabolic governing equations must use a marching approach along the channel that does have influences from downstream, and therefore cannot be used to predict reverse flow. Comprehensive comparisons with work of Najim et al. [29] and the parabolic approach used by Tohidi and Ormiston [32] (i.e., the results in Chapter 5) are performed to illustrate the capability of the elliptic approach to model the evaporation process. A new set of detailed results, including the effects of liquid and mixture Reynolds number changes on flow, heat, and mass characteristics during the evaporation process are also presented.

6.1.1 Problem statement

A diagram of the physical model considered in this study is shown in Figure 6.1. A fully devel-

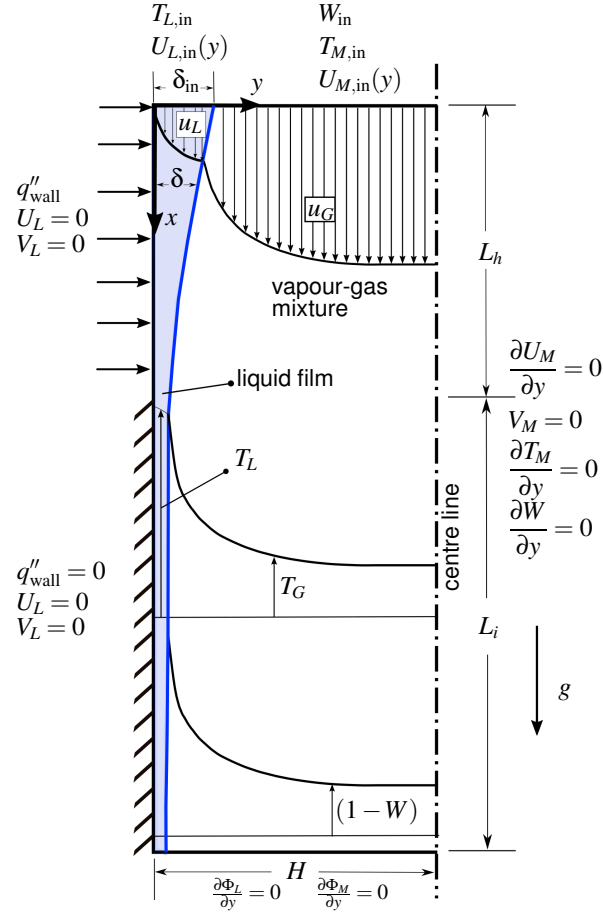


Figure 6.1: Domain definition and boundary conditions for two-phase evaporation in a vertical channel

oped two-phase laminar flow of a gas-vapour mixture and pure liquid flows downward in a vertical channel with a half width of H and length of L . The liquid film with uniform inlet temperature enters the channel with initial thickness of δ_{in} . The gas-vapour mixture enters with uniform temperature and gas mass fraction. The inlet axial velocities of both the film and mixture are specified by a fully developed profile; the transverse velocities are zero. The liquid is flowing over a wall including a heated entry section and an insulated exit section. A partially heated channel was used

to enable recirculation zones to be seen while avoiding flow reversal at the channel exit. The liquid film thickness decreases along the channel at the heated section (L_h) due to mass removal, and it remains almost constant along the insulated section (L_i).

6.2 Grid independence study

A grid independence study was conducted using a typical case studied in this work (Case W8 described in Section 6.4). The range of the number of nodes in these tests were as follows: $10 \leq N_{y,L} \leq 30$, $40 \leq N_{y,M} \leq 140$, and $105 \leq N_x \leq 400$. The transverse profiles for the velocity, temperature, and air mass fraction at the channel exit were compared for different grids. Comparing with the finest grid ($N_{y,L} = 30$, $N_{y,M} = 140$, and $N_x = 400$), a grid with $N_{y,L} = 20$, $N_{y,M} = 70$, and $N_x = 210$ had the maximum percent differences of 0.15, 0.03, and 0.02 for velocity, temperature, and air mass fraction, respectively. These differences are considered to be sufficiently small, so the above-mentioned grid was used for all the results presented in this work.

6.3 Comparisons with previous works

In this section, the results of the present model are compared to the two earlier works that studied the evaporation of air-water inside vertical parallel plate channels with uniform heated walls and no insulated sections. In the first step, the results of the current elliptic model are compared against those of Najim et al. [29] who used a marching scheme in their simulations. In the second step, the results are compared with one of the cases studied by Tohidi and Ormiston [32] who also used a marching scheme. Table 6.1 summarizes the operating parameters of the comparison cases.

Figure 6.2 compares the results of the present study to results presented by Najim et al. [29]. A comparison has been made for the film thickness along the channel and for the velocity, temperature, and vapour mass fraction in the transverse direction at the channel exit. It was observed

Table 6.1: Definitions of comparison cases

Case	Authors	$Re_{M,in}$	$Re_{L,in}$	$Fr_{L,in}$	$T_{L,in}$ [°C]	$T_{M,in}$ [°C]	q''_{wall} [W/m ²]
W1	[29]	100	44.8	3.66	25	25	8000
W2	[32]	2000	50	4.18	20	20	500

that the mixture was supersaturated in the region close to the channel exit, where the relative humidity was as high as 105%. Therefore, the code has been run with and without the EMC model to investigate the effects of excess moisture on the field variables. As seen in Fig. 5.1, the excess moisture does not affect the velocity, film thickness and temperature; however, it has an impact on the vapour mass fraction, which decreases when using the EMC model. When the EMC model is off, the mass fraction distribution is also in good agreement with that presented by Najim et al. For all variables, the trends of the results are similar, and the small differences between the results can be due to the differences between the equations, solution procedure, and calculation of the film thickness and pressure. The difference in the calculation of thermophysical properties could also contribute to the deviations. Over the gas phase, the maximum percent differences between the current work and Najim et al. [29] are 9.93%, 1.38%, and 0.09% for velocity, film thickness, and temperature, respectively, when using the EMC model. The maximum percent difference for the vapour mass fraction is 3.76% and 0.54% with and without using the EMC model, respectively.

The present results were also compared to Tohidi and Ormiston [32] for Case W2. In this test case the relative humidity never exceeds 100%, so the results of the code with and without the EMC model are identical. The results of heat transfer, the film thickness, and outlet temperature and mass fraction of the present work are in excellent agreement with those of the parabolic approach used by Tohidi and Ormiston. The maximum percent differences between the present study and the parabolic results are 0.1% and 7.38%, 0.055% and 0.029% for the interface, heat flux, temperature, and mass fraction, respectively.

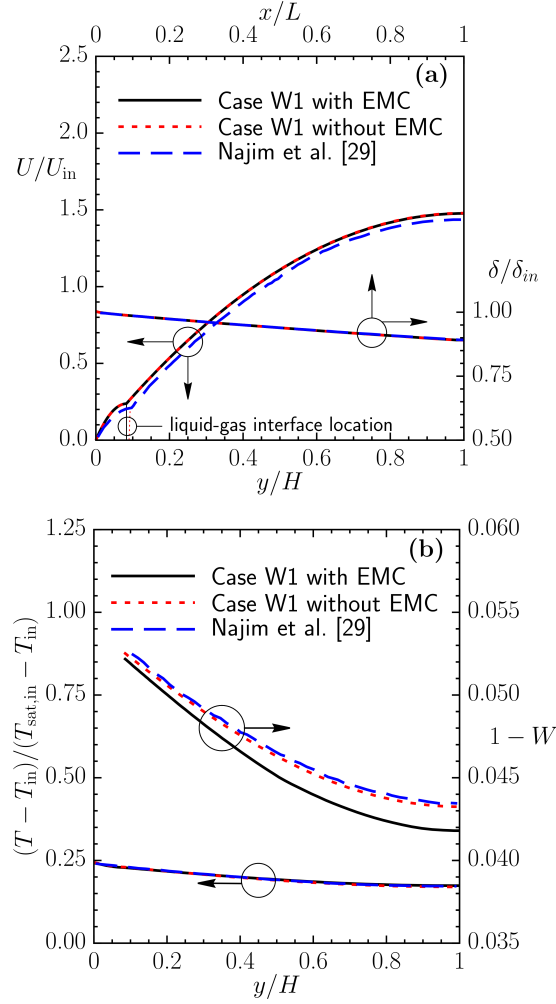


Figure 6.2: Case W1 comparison of (a) velocity and film thickness and (b) temperature and vapour mass fraction

The good agreement with previous numerical studies demonstrates the accuracy and reliability of the present elliptic model. The model will now be used for a detailed investigation of aspects of falling film evaporation and the effects of buoyancy forces on the flow and thermal characteristics of the system for the partially heated channel shown in Figure 6.1.

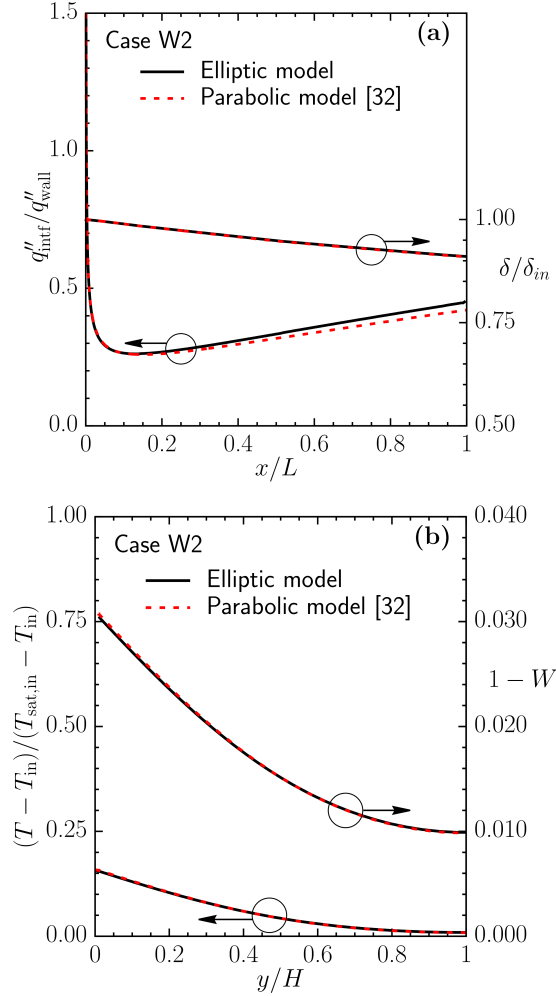


Figure 6.3: Case W2 comparison of elliptic equation model and parabolic equation model results for (a) film thickness and interfacial heat flux and (b) temperature and vapour mass fraction

6.4 Results and discussion

The common input parameters for all simulations in this section are: $L_h = 0.3$ m, $L_i = 0.7$ m, $H = 0.015$ m, $q''_{\text{wall}} = 3000$ W/m², $T_{L,\text{in}} = 20^\circ\text{C}$, $T_{M,\text{in}} = 20^\circ\text{C}$, $P_{\text{in}} = 1$ atm, and $\phi_{\text{in}} = 50\%$. The inlet liquid Reynolds number was either 25 or 35. The range of inlet mixture Reynolds numbers was from 200 to 800. Table 6.2 indicates the operating parameters for parametric study cases. The cases will be used to study the effects of $\text{Re}_{L,\text{in}}$ and $\text{Re}_{M,\text{in}}$ on the flow and thermal characteristics

of the system. Grashof numbers and reverse flow will be discussed later.

Table 6.2: Parametric study cases for water

Case	$Re_{L,in}$	$Fr_{L,in}$	$Re_{M,in}$	$\overline{Gr}_T$	$\overline{Gr}_M$	Reverse Flow	Location [m] ¹
W3	25	2.081	200	173.53	68.81	Yes	0.181
W4	35	2.914	200	132.31	47.28	Yes	0.260
W5	25	2.082	400	160.27	61.06	Yes	0.306
W6	35	2.915	400	125.11	44.07	No	-
W7	25	2.084	800	147.14	53.96	No	-
W8	35	2.917	800	117.20	40.78	No	-

¹ Axial location where the flow reversal is initiated.

In order to demonstrate the impacts of the supersaturation phenomenon on the field variables, results for Case W7 with and without the excess moisture condensation model are presented. Case W7 was selected because it has the highest evaporation rate among those in the parametric study.

Figure 6.4 illustrates the distribution of the relative humidity in the domain with and without the EMC model. Before using the EMC model, the area near the interface becomes supersaturated after $X=0.2$, and the relative humidity increases up to a maximum value of 115% along the channel. This excess vapour could affect the field variables in the system. As is seen in Figure 6.4b, the excess water vapour is removed from the system after using the EMC model, and the relative humidity is less than or equal to 100% everywhere, showing the capability of the EMC model to avoid the supersaturation phenomenon in the system.

The transverse variation of the relative humidity at the channel exit is presented in Figure 6.5a. The mixture is supersaturated at the channel exit before using the EMC model, and the relative humidity experiences a peak at the mid-width of the channel. The EMC model keeps it under saturation by removing the excess moisture from the domain. Figure 6.5b shows the U velocity

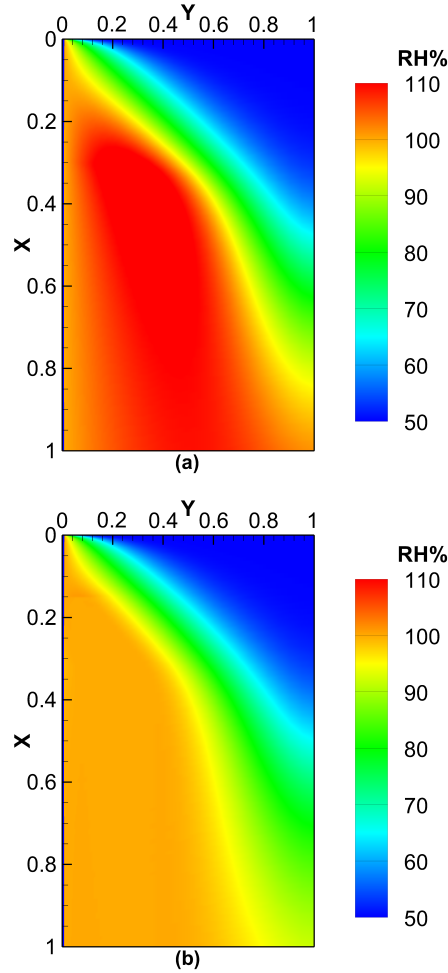


Figure 6.4: Relative humidity distribution in the domain (not to scale) for Case W7 (a) without EMC model, (b) with EMC model

profile in the transverse direction at the channel exit for Case W7 with and without the EMC model. The use of the EMC model does not affect the velocity profile significantly. The difference between the two cases is due to the condensation of vapour in the region near the interface leading to a slight reduction of opposing mass buoyancy force which increases the velocity near the interface. The velocity also decreases close to the centre line to conserve the mass crossing the axial location.

Figure 6.6 presents the effects on the mass fraction and temperature at the channel exit when

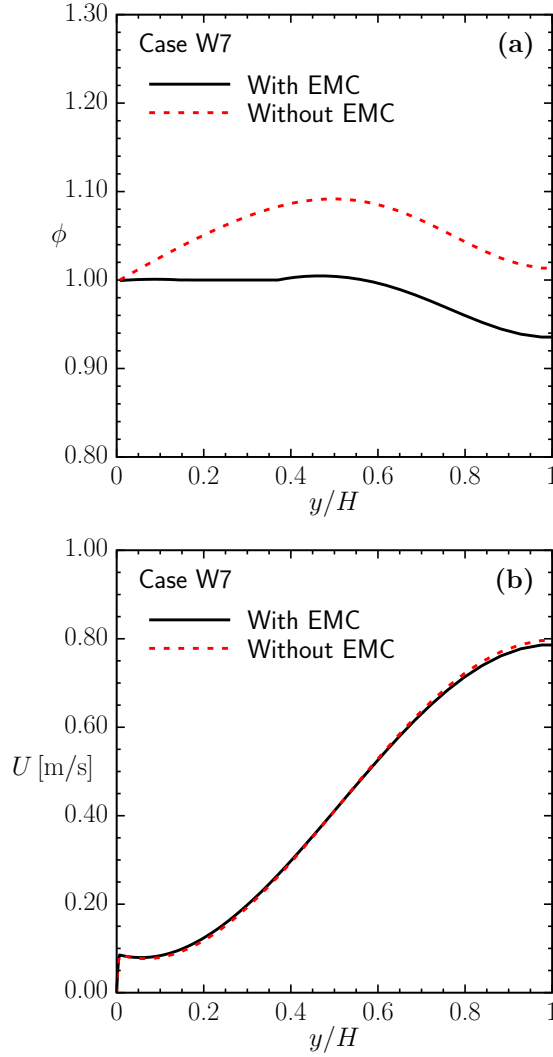


Figure 6.5: Case W7 transverse variation at the channel exit of (a) relative humidity (b) U velocity

using the EMC model. The mass fraction increases by using the EMC model, as is seen in Figure 6.6a. The EMC model removes the excess water vapour from the mixture and keeps the relative humidity less than 100% leading to a higher air mass fraction in the system. The temperature decreases slightly, as shown in Figure 6.6b, which is due to the energy removed by the moisture condensation and the temperature adjustment to have a lower saturation pressure and relative humidity. The maximum percent difference for the mass fraction and temperature at the outlet are

0.34 and 0.37, respectively. These differences are corresponding to about 10% supersaturation.

For Case W7, it was observed that the amount of condensed mass is only 2.05% of evaporated mass in the entire system and is about 0.1% of the inlet liquid mass flow rate. The EMC model is used for the rest of the results presented in this study.

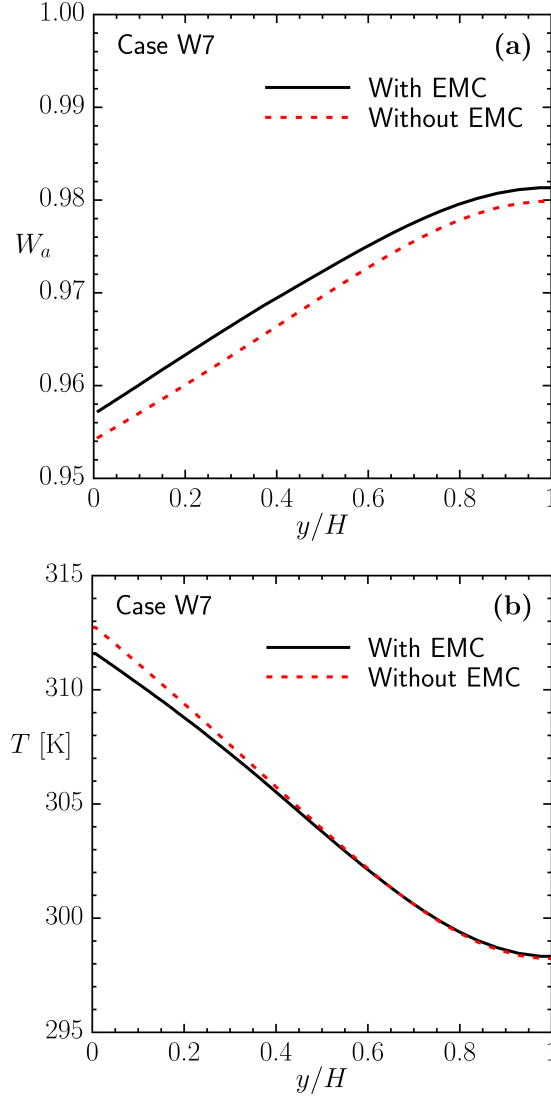


Figure 6.6: Case W7 transverse variation at the channel exit of (a) air mass fraction, (b) temperature

Inside a channel with downward inlet flow, locally the gas-phase flow can move upwards or downwards, depending on the directions of the shear, thermal buoyancy, and solutal buoyancy

forces. In a system with a forced convection co-current flow, the interfacial shear force always acts downwards (aiding). The thermal buoyancy force is opposing and acts upwards when energy is added to the mixture, and the interface temperature is higher than the mixture temperature. Depending on the molecular weight of the liquid relative to the air, the solutal buoyancy force can act either upwards or downwards. If the molecular weight of the liquid is less than the air, the solutal buoyancy acts upwards (opposing); otherwise, it acts downwards (aiding). For water, the solutal buoyancy always acts upwards because the molecular weight of water is less than that of the air. Therefore, thermal and solutal buoyancy forces can significantly affect the flow characteristics in a case where the forced convection effects are not very strong. In order to measure the thermal and solutal buoyancy forces, the local Grashof numbers are defined based on the interface temperature and mass fraction:

$$\text{Gr}_T = \frac{g (T_{\text{intf}} - T_{M,\text{in}}) H^4}{L v_M^2 T_{M,\text{in}}} \quad (6.1)$$

$$\text{Gr}_M = \frac{g (M_a/M_v - 1) (W_{a,\text{in}} - W_{a,\text{intf}}) H^4}{L v_M^2} \quad (6.2)$$

Average Grashof numbers can also be defined as:

$$\overline{\text{Gr}}_T = \frac{1}{L} \int_0^L \text{Gr}_T dx \quad (6.3)$$

$$\overline{\text{Gr}}_M = \frac{1}{L} \int_0^L \text{Gr}_M dx \quad (6.4)$$

Figure 6.7 illustrates the change of thermal and mass Grashof numbers along the channel length for cases with different $\text{Re}_{M,\text{in}}$. For the heated section (up to $x/L=0.3$), the buoyancy forces are increasing due to the increase in the evaporation rate along the channel. The buoyancy forces decrease in the insulated section, however, which is due to the decrease in the temperature and vapour mass fraction at the interface. For the insulated section, no energy is added to the system, so the interfacial temperature decreases along the channel. Moreover, the air gradually diffuses towards the interface reducing the interfacial vapour mass fraction and consequently the mass Grashof number. The average Grashof numbers for Cases W3 to W8 are listed in Table 5.2. Both

Grashof numbers decrease by increasing $Re_{L,in}$ which is due to the reduction of the evaporation rate. A higher liquid mass flow rate raises the amount of the energy required for heating the liquid film, which results in a lower interfacial temperature at a fixed wall heat flux. Furthermore, the advected energy by the liquid along the channel increases for higher liquid flow rates, decreasing the amount of latent heat transfer and the evaporation rate. As seen in Table 5.2, both thermal and mass Grashof numbers are positive, meaning that the buoyancy forces are opposing the flow direction.

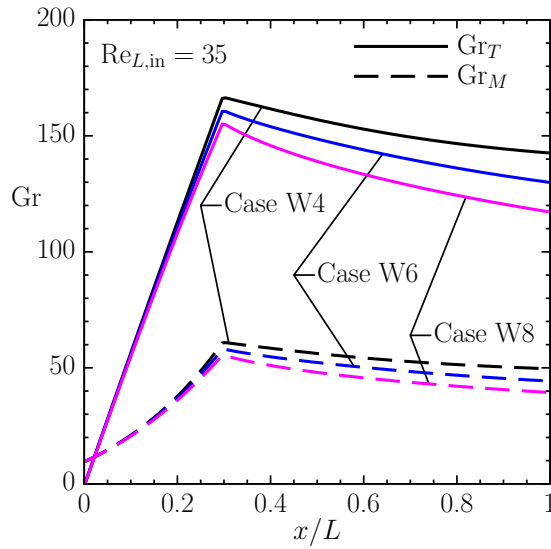


Figure 6.7: Axial variation of thermal and mass Grashof numbers for different mixture inlet Reynolds numbers

Figure 6.8 presents the U velocity change in the transverse direction at the middle ($x/L=0.5$) and the outlet ($x/L=1.0$) in the channel. The inlet average velocity values used to normalize the velocity were 0.1014, 0.1015, 0.203 and 0.406 m/s for Cases W3, W4, W6, and W8, respectively. The velocity is positive for all cases at the channel exit, indicating that no reverse flow occurs at the outlet. In the middle of the channel, however, the negative velocity is observed for Cases W3 and W4 in the mixture region near the interface, which illustrates that the opposing forces play a dominant role in the system. For the lowest $Re_{M,in}$, the buoyancy forces overcome the

aiding forces, causing a flow reversal in the domain. Moreover, the evaporation rate is higher for the lower $Re_{L,in}$ leading to higher heat and mass transfer rate and consequently to more powerful buoyancy forces.

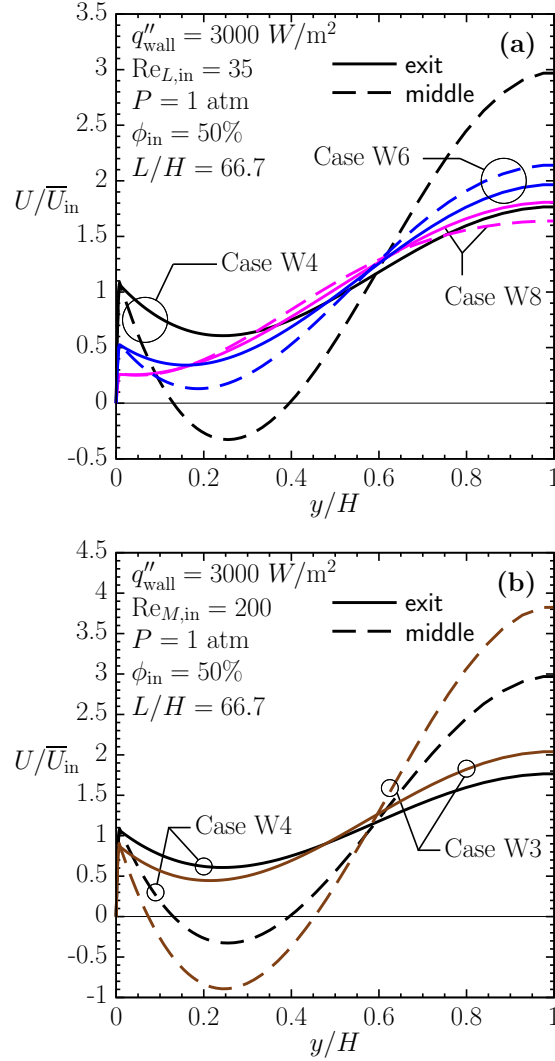


Figure 6.8: Transverse U velocity distribution at the middle and outlet of the channel for (a) $Re_{M,in} = 200, 400$, and 800 for Cases W4, W6, and W8, respectively and (b) $Re_{L,in} = 25$ and 35 for Cases W3 and W4, respectively

Figure 6.9 shows a part of the domain for Case W3 in which the flow reversal starts to form

near the interface. The upward streamlines are observed after the midpoint of the heated section, indicating the strength of the buoyancy forces in the system. The reverse flow occurs near the interface due to the liquid film evaporation and the high rate of the air replacement with the water vapour in that region.

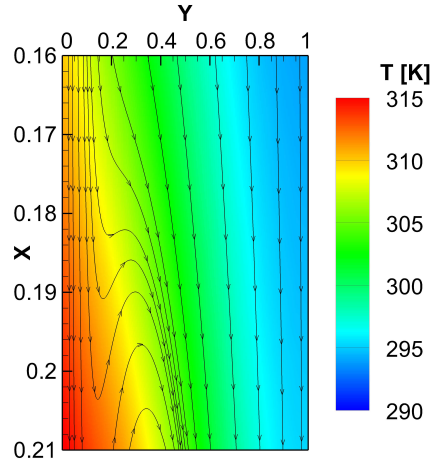


Figure 6.9: Streamlines in a part of domain (not to scale) where the flow reversal is observed (Case W3)

The axial locations in which the negative U velocity component is initiated are listed in Table 5.2. For Cases W6 to W8, no flow reversal occurs because there is strong forced convection. For Cases W5 and W6, the flow pattern depends on $Re_{L,in}$, which directly affects the evaporation rate. Because the amount of energy needed for heating the liquid film decreases by reducing the liquid mass flow rate, a lower value of $Re_{L,in}$ results in a higher evaporation rate, which increases the interfacial temperature and the amount of water vapour in the system. For case W5, the higher evaporation rate leads to stronger buoyancy forces, causing the flow reversal in the system. For Case W5, the flow reversal occurs after the heated section because just after the heated zone the temperature difference between the liquid film and the gas is still high enough to produce the evaporation, leading to the dominance of the buoyancy forces in the insulated section. For Cases W3 and W4, the shear force is smaller, resulting in the most substantial flow reversal among the studied

cases. For cases with more powerful buoyancy forces (Cases W3 and W4), the location where the negative velocities are initiated is shifted closer to the channel inlet.

The presence of the insulated section affects the flow patterns dramatically. Because the evaporation process almost stops in the region far from the heated section, the interfacial temperature decreases along the channel. Also, the water vapour is gradually replaced with air near the interface. Because the air is heavier than the water vapour, the aiding solutal buoyancy and shear forces become dominant again, making the flow direction positive. The interaction of shear and buoyancy forces leads to the creation of recirculation zones in cases where the flow reversal occurs. The recirculation phenomenon can be further understood by tracking the local Grashof numbers along the channel length. As indicated in Figure 6.7, the Grashof numbers decrease after the heated section, suggesting that the forced convection overcomes the natural convection again.

The flow streamlines for all cases listed in Table 5.2 are presented in Figure 6.10. The distance between the location where the negative velocities are initiated and the channel inlet provides an indication of the strength of the opposing forces in the system. For example, for Case W3, negative velocities are initiated at $X = 0.181$, and for Cases W4 and W5, the location is at $X = 0.260$ and $X = 0.306$, respectively. For Case W3, the largest recirculation zone is formed. For the cases having a recirculation zone, the mixture temperature is higher. This higher temperature occurs because the water vapour produced at the interface recirculates and transfers energy towards the channel centre line, resulting in a higher temperature in the mixture region. Furthermore, the size of a recirculation zone indicates its power to transfer energy and mass to the other parts of the system. Hence, Case W3 is capable of transferring more energy than other cases to other parts of the system which causes a noticeable temperature increase in the mixture.

Figure 6.11a presents the interfacial heat flux for different mixture Reynolds numbers at $Re_{L,in} = 35$. After the heated zone, the evaporation rate is low, and the temperature gradient at the interface is not significant, so the heat flux approaches a negligible value at the end of the insulated section. A higher $Re_{M,in}$ results in a higher capacity to carry the energy away from the interface. Moreover,

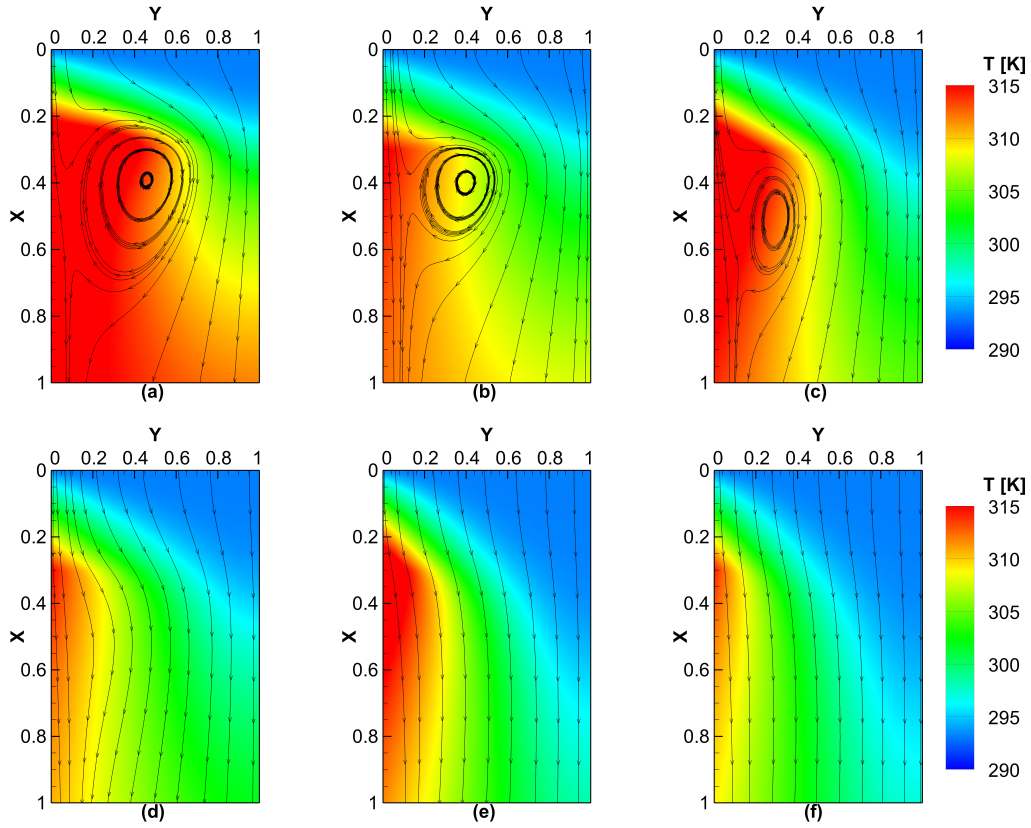


Figure 6.10: Flow streamlines (not to scale) for different cases (a) W3, (b) W4, (c) W5, (d) W6, (e) W7, (f) W8

the mass transfer coefficient increases by increasing the gas velocity leading to a higher evaporation rate at higher mixture Re numbers. For cases with $Re_{L,in} = 25$ (Figure 6.11b), the higher evaporation rate and interface temperature lead to a higher amount of heat transfer at the interface. For Case W3, the creation of the recirculation zone affects the interfacial heat flux at the heated section, and the trend is different from other cases having the recirculation zone (Cases W4 and W5). Case W3 experiences a heat flux decrease in the middle of the heated zone, which is due to the strong flow reversal close to the interface (see Figure 6.10a). Cases W3 and W5 also show an increase of interfacial heat flux at the insulated section which is not observed for the case with the same $Re_{M,in}$ number (Cases W4 and W6). Thus, it can be concluded that the strong recirculated

flow can increase the interfacial heat transfer at the insulated section which can be due to the higher temperature in the mixture region and the energy transported upstream from the mixture flow.

Figure 6.12 shows the interfacial mass flux along the channel length. The mass flux shows the same trends as that of the heat flux at the interface. This figure indicates that for Case W3, the evaporation rate is negatively affected by the reverse flow at the heated section, but it increases at the beginning of the insulated section.

As stated in the previous study [32], the effectiveness is defined as the ratio of the total evaporation mass flow rate to the mass flow rate that could be evaporated based on the per unit depth total wall heat transfer rate and latent heat of vaporization.

$$\varepsilon = \frac{\dot{m}'_{L,in} - \dot{m}'_{L,out}}{\left(\frac{q''_{wall} L_h}{h_{fg}} \right)} \times 100 \quad (6.5)$$

For the calculation of ε , h_{fg} was evaluated at the channel inlet conditions. Figure 6.13a illustrates the effectiveness of a system for different $Re_{L,in}$ and $Re_{M,in}$ numbers. As expected, the effectiveness increases by reducing the liquid Reynolds number because a higher portion of energy is used for the phase change in the lower liquid Reynolds numbers. The effectiveness of the system increases 31.9% when changing the the liquid Reynolds number from 35 to 25 at $Re_{M,in} = 800$. The effectiveness also increases by increasing the mixture Reynolds number due to the higher evaporation rate at higher $Re_{M,in}$. The effectiveness increases by 31.2% when $Re_{M,in}$ changes from 200 to 800 at $Re_{L,in} = 25$.

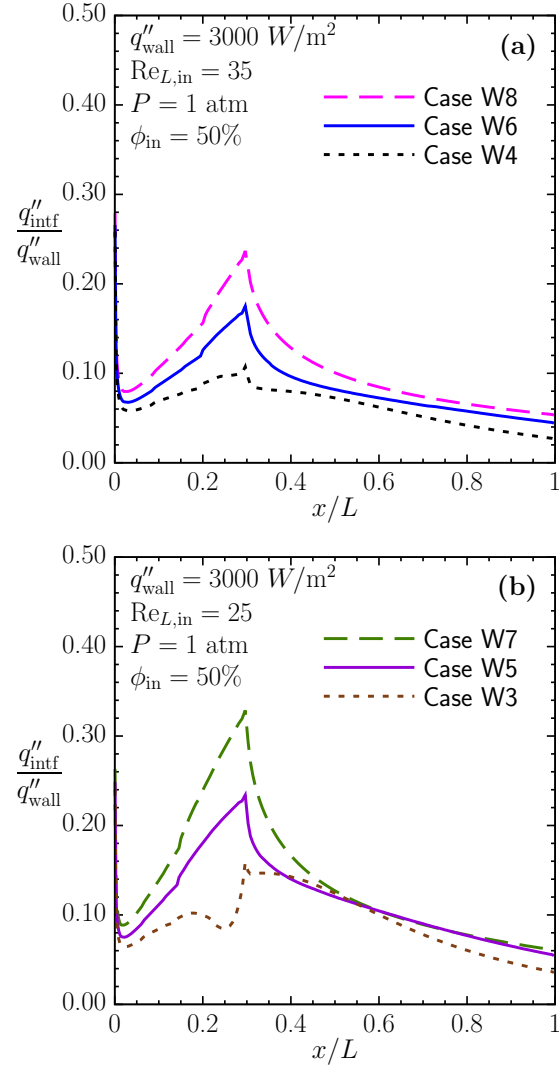


Figure 6.11: Axial variation of interfacial heat flux for different $\text{Re}_{M,\text{in}}$ numbers at (a) $\text{Re}_{L,\text{in}} = 35$, (b) $\text{Re}_{L,\text{in}} = 25$

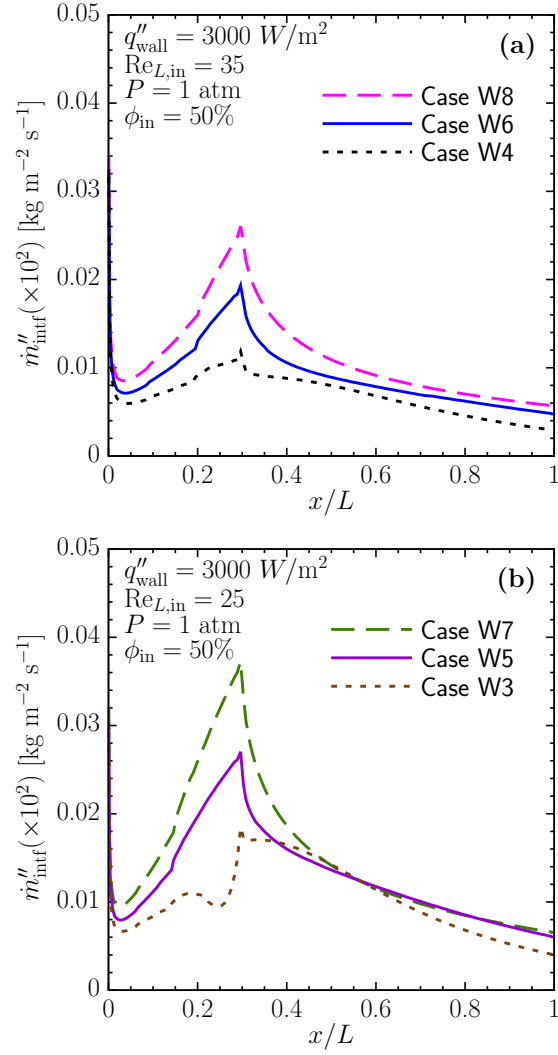


Figure 6.12: Axial variation of interfacial mass flux for different $\text{Re}_{M,\text{in}}$ numbers at (a) $\text{Re}_{L,\text{in}} = 35$ and (b) $\text{Re}_{L,\text{in}} = 25$

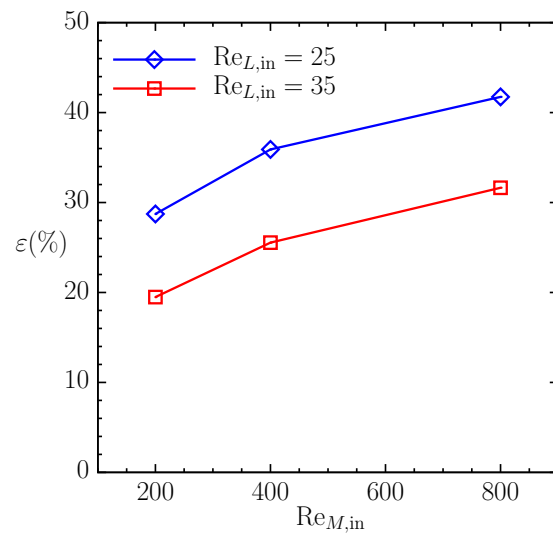


Figure 6.13: Effectiveness variation for different inlet liquid and mixture Reynolds numbers

Chapter 7

Desalination Process inside Parallel-Plate Channels: Elliptic Model

7.1 Introduction

In this chapter, an in-house code is utilized to simulate the evaporation of fresh water and salt water falling film in a vertical parallel plate channel. To the best knowledge of the author, the implementation of an elliptic approach to a two-phase falling film desalination process inside a vertical parallel plate channel has not been previously addressed. The main objective of the present study is to numerically investigate the effects of mixed convection and salt concentration on the flow and thermal characteristics of the evaporation process of liquid saline water film within a vertical parallel plate channel. The validity of the present model was assessed through comparisons with a previous experimental study for pure water evaporation [1]. One of the new features in this work is the partial enthalpy related transport advection in the liquid energy conservation equation that has not been considered in the previous desalination studies. Also, the performance of this new model is illustrated by studying the impacts of inlet liquid Reynolds number, wall heat flux, salinity, and air relative humidity on the details of the flow and heat and mass transfer for falling film thermal desalination in a vertical parallel plate channel.

7.2 Problem Statement

A representation of the computational domain is depicted in Figure 2.1. The liquid film mixture enters with an initial thickness of δ_{in} , a fully developed profile for the axial velocity, $U_{L,in}(y)$, and uniform profiles for the inlet temperature, $T_{L,in}$, and salt mass fraction, $W_{S,in}$. The film flows along

the wall exposed to a uniform heat flux, q''_{wall} . The gas mixture enters with a fully developed profile for the axial velocity, $U_{M,\text{in}}(y)$, and uniform profiles for the mixture temperature, $T_{M,\text{in}}$, and the air mass fraction, $W_{a,\text{in}}$.

7.3 Grid independence study

Case SW3, described in Section 7.5, was selected for the grid independence study. Various sets of node numbers, N , were tested within the following ranges: $10 \leq N_{y,L} \leq 40$, $30 \leq N_{y,M} \leq 120$, and $90 \leq N_x \leq 300$. The outlet y -direction profiles of the axial velocity, the temperature, and the air mass fraction were compared for numerous grids. A grid with $N_{y,L} = 20$, $N_{y,M} = 70$, and $N_x = 180$ was found to be suitable because the maximum percent difference between its results and those for the finest grid ($N_{y,L} = 40$, $N_{y,M} = 120$, and $N_x = 300$) were 0.026, 0.37, and 0.88 for temperature, mass fraction, and axial velocity, respectively. Because these differences are adequately small, the grid with $N_{y,L} = 20$, $N_{y,M} = 70$, and $N_x = 180$ was used to produce the results in this study.

7.4 Comparisons with a previous experimental study

The results from the present model were compared to the experimental results presented by Yan et al. [1] who examined the evaporation from pure water to humid air in an insulated vertical parallel plate channel. The operating parameters in their work are: $\dot{m}'_{L,\text{in}} = 0.04$ to $0.06 \frac{\text{kg}}{\text{m.s}}$, $T_{L,\text{in}} = 50 \text{ }^\circ\text{C}$, $T_{M,\text{in}} = 30.5 \text{ }^\circ\text{C}$, $P_{\text{ref},\text{in}} = 1 \text{ atm}$, $q''_{\text{wall}} = 0 \text{ W/m}^2$, $\phi = 85\%$, $L = 1.0 \text{ m}$, and $H = 0.015 \text{ m}$. As mentioned in their work, the measurement of the velocity distribution in the gas phase was difficult. Therefore, no information regarding the inlet mixture Reynolds number was provided. In the present study, simulations were performed with $\text{Re}_{M,\text{in}}$ values of 500, 1000, and 2000. Figure 7.1 shows the wall temperature distribution along the channel for two different inlet liquid mass flow rates. The maximum percent difference between $\text{Re}_{M,\text{in}} = 500$ and $\text{Re}_{M,\text{in}} = 2000$ occurs at the

channel exit and is equal to 3.1 and 2.2 for the inlet liquid mass flow rate of 0.04 and 0.06 $\frac{\text{kg}}{\text{m.s}}$, respectively. Hence, the effect of $\text{Re}_{M,\text{in}}$ on the wall temperature distribution is not considerable for different $\dot{m}'_{L,\text{in}}$ values. Yet, as is seen in Figure 7.1, the results corresponding to $\text{Re}_{M,\text{in}} = 1000$ shows a better agreement with the measurement, and the highest deviation for this Reynolds number occurs close to the channel inlet with a maximum percent differences of 1.15 and 0.87 for $\dot{m}'_{L,\text{in}} = 0.04$ and 0.06 $\frac{\text{kg}}{\text{m.s}}$, respectively. This good agreement illustrates the validity of the present numerical model for evaporation modelling.

7.5 Results and discussion

The parameters that are common for all parametric study simulations are: $L = 1.0$ m, $H = 0.015$ m, $\text{Re}_{M,\text{in}} = 2000$, $T_{L,\text{in}} = 20^\circ\text{C}$, $T_{M,\text{in}} = 20^\circ\text{C}$, $P_{\text{ref},\text{in}} = 1$ atm, and inlet relative humidity $\phi_{\text{in}} = 50\%$ ($W_{a,\text{in}} = 0.993$). In the parametric study, the liquid inlet Reynolds value, $\text{Re}_{L,\text{in}}$, was 25 or 35, and the wall heat flux, q''_{wall} , was 2000 or 4000 W/m^2 . The oceanographic range of salinity, S , is usually from 0 to 40 g/kg; however, the salinity might be higher in some areas due to a high evaporation rate and little fresh water inflow. For example, it can be up to 50 g/kg in the Persian Gulf water or reach a value of 70 g/kg in Australian Shark Bay. Hence, in the present study, a salinity range of 0 to 70 g/kg was studied. Table 7.1 lists the parametric study cases. In the present work, the effects of changing $W_{S,\text{in}}$, $\text{Re}_{L,\text{in}}$, and q''_{wall} on the flow, the heat transfer, and the mass transfer were studied. Also, the impacts of air relative humidity on the field variables and evaporation rate were investigated for one case. The EMC model presented by Tohidi and Ormiston [33] was active in all simulations. In Table 7.1, the liquid froude number is defined as $\text{Fr}_L = \overline{U}_{L,\text{in}}^2 / (g\delta_{\text{in}})$.

Figure 7.2 shows the y-direction profiles of the axial velocity, U , in both phases at different axial locations. The non-dimensional transverse-direction coordinate, η , as defined in [106], is used in Figures 7.2 to 7.4, where the ranges $0 \leq \eta \leq 1$ and $1 \leq \eta \leq 2$ represent the liquid and gas phases, respectively. As seen in Figure 7.2, the liquid film velocity changes very little axially for all cases considered. Close to the interface in the gas region, the velocity is reduced along the channel

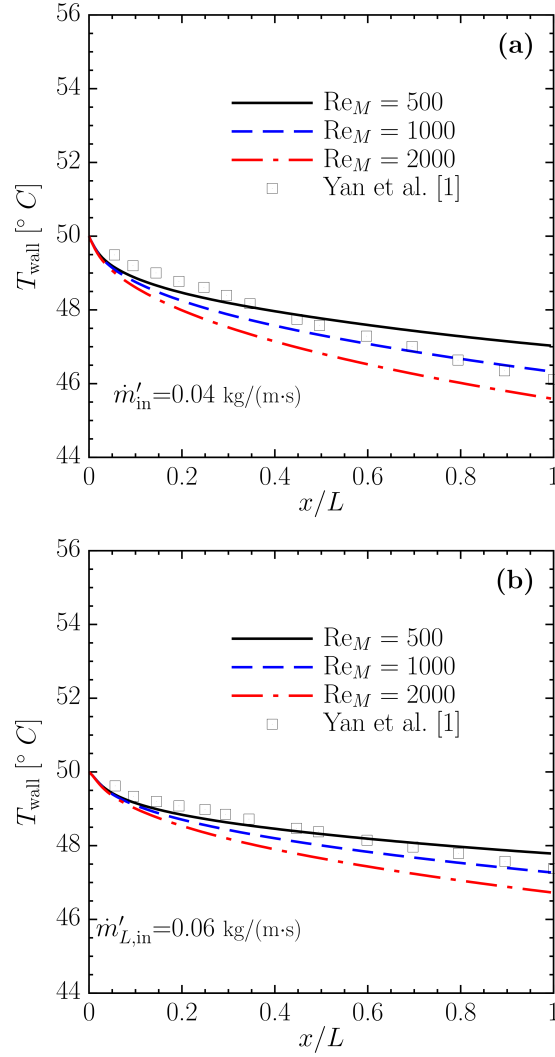


Figure 7.1: Comparison of wall temperature distribution against experimental data [1] (a) $\dot{m}'_{L,\text{in}} = 0.04 \frac{\text{kg}}{\text{m}\cdot\text{s}}$ and (b) $\dot{m}'_{L,\text{in}} = 0.06 \frac{\text{kg}}{\text{m}\cdot\text{s}}$

because of the evaporation process and increasing water vapour in that region. Replacing the air with water vapour near the interface yields a lighter mixture and an opposing buoyancy force. Increases in the interfacial temperature and water vapour mass fraction augment the thermal and mass opposing buoyancy forces, respectively, which affect the axial velocity close to the interface. In addition, the gas phase velocity increases slightly with increasing the salinity close to the centre

Table 7.1: Definitions of cases for pure water and salt-water

Case	$Re_{L,in}$	$Fr_{L,in}$	q''_{wall} [W/m ²]	$W_{S,in}$ [g/kg]
W1	25	2.09	2000	-
W2	25	2.09	4000	-
W3	35	2.92	2000	-
W4	35	2.92	4000	-
SW1	25	2.09	2000	35
SW2	25	2.09	2000	70
SW3	25	2.09	4000	35
SW4	25	2.09	4000	70
SW5	35	2.92	2000	35
SW6	35	2.92	2000	70
SW7	35	2.92	4000	35
SW8	35	2.92	4000	70

line. That increase occurs because the inlet film thickness increases with increasing the amount of salt in the liquid mixture leading to a reduced gas section width. For constant $Re_{L,in}$ and $Re_{M,in}$, the reduced width results a velocity increase in the gas phase.

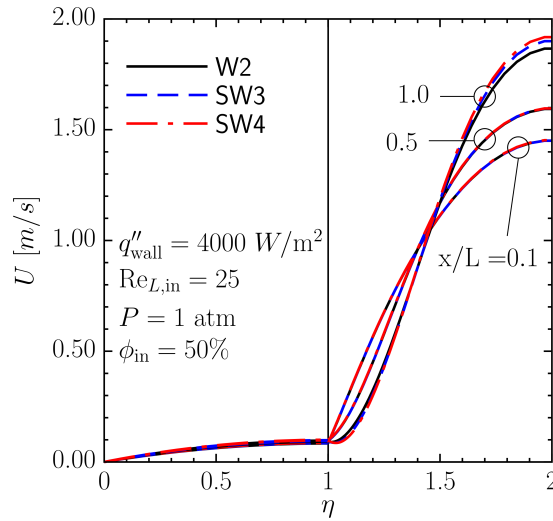


Figure 7.2: U velocity distribution in transverse direction at different axial locations

Figure 7.3 depicts the temperature distribution in the transverse direction at different axial

locations. The constant wall heat flux increases the liquid temperature along the channel. In the transverse direction, the temperature decreases from the wall to the interface in the liquid phase, indicating the direction of liquid sensible heat transfer is from the wall to the interface. The temperature also decreases from the interface to the centre line in the gas phase region. The effect of salinity on the liquid temperature is not significant close to the inlet. However, the effect of salinity on the temperature distribution increases along the channel. The temperature increase with the salinity is more noticeable at the channel exit because the total energy added to the both phases is significant at the channel exit, causing the salt mass fraction to increase in the liquid film at a higher rate. The specific heat of salt-water is lower than that of pure water, indicating a lower capacity of salt-water to store heat. The heat transfer between the wall and the flow increases the energy of the system, which is eventually absorbed by the flow as enthalpy. Consequently, enthalpy increases from the inlet to the outlet. For a lower specific heat, the increase in enthalpy along the channel results in a larger temperature increase in the liquid film. At the channel exit, the wall temperature increases about 7.5 K from Case W2 to SW4. Boiling point elevation refers to the increase in the interface saturation temperature, which corresponds to the vapor partial pressure, resulting from the presence of salt in the liquid. The increase of the liquid temperature along with the boiling point elevation of salt-water cause a temperature increase at the interface and gas region with high salinity values.

Figure 7.4 a presents the salt concentration mass fraction change in the liquid phase at different axial locations, for Cases SW3 and SW4. The average salt mass fraction increase from the inlet to the channel exit is 18.6% and 16.4% for Cases SW3 and SW4, respectively. As evaporation occurs, water leaves the liquid film, but the amount of salt remains intact in the liquid leading to a higher salt concentration at the outlet. A salt concentration accumulated at the interface is observed close to the interface that occurs due to the water evaporation and salt impermeability to the gas phase at the interface. The water vapour mass fraction distribution in the gas phase is depicted in Figure 7.4 b. The vapour mass fraction increases axially because of evaporation. The wall heat flux constantly adds energy to the liquid phase and that energy is transferred to the interface to

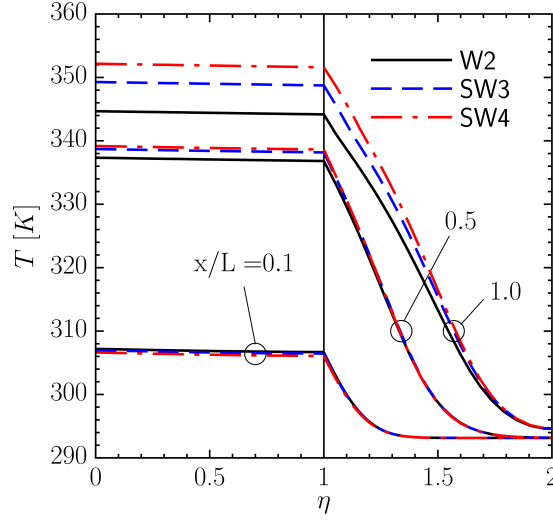


Figure 7.3: Temperature distribution in transverse direction at different axial locations

enhance the evaporation rate. The vapour concentration is maximum at the interface and decreases towards the centre line. The amount of the vapour increases close to the interface because of a high rate of evaporation and replacement of air with water vapour in that region. The amount of vapour is not affected by the salinity at the inlet and middle of the channel; however, its interfacial value increases about 10% from Case SW3 to Case SW4. This increase can be due to the interfacial temperature increase, discussed earlier, which affects the saturation pressure and consequently the inlet vapour mass fraction. The vapour mass fraction decreases towards the centre line where it is nearly the same for different salinity values.

The axial variation of the interface temperature is shown in Figure 7.5. The interfacial temperature increases along the channel because of the constant rate of energy added to the system. The interface temperature also increases more with higher inlet salinity. Compared to $T_{L,in}$, the interfacial temperature increases by about 51, 55.5 and 58.5 K at the channel exit for Cases W2, SW3 and SW4, respectively. This temperature increase can be attributed to the boiling point elevation of salt-water, along with its lower specific heat and latent heat compared to pure water, resulting in the transfer of more energy as sensible heat in the system as the salinity increases.

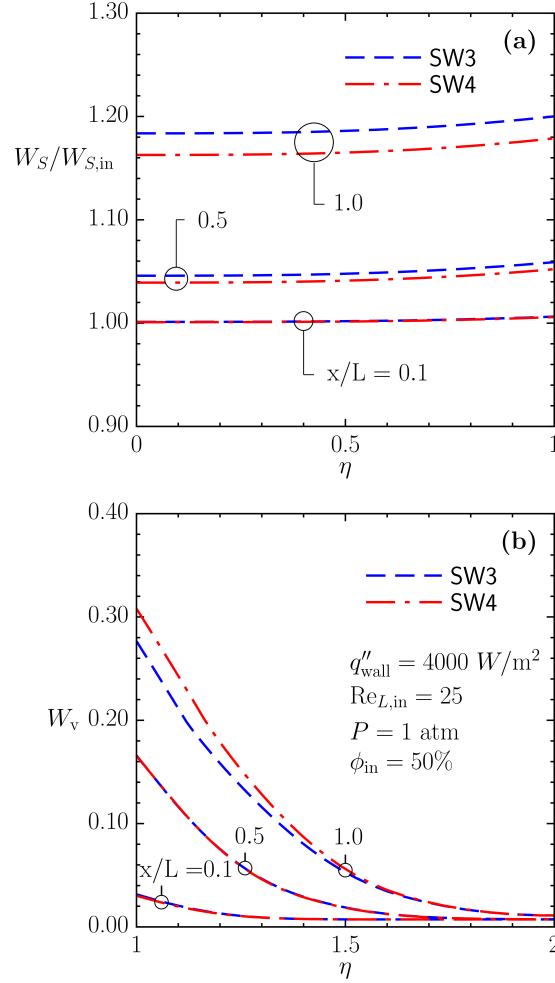


Figure 7.4: (a) Salt and (b) water vapour mass fraction change with salinity in the transverse direction at different axial locations

The axial variations of the interfacial salt mass fraction relative to the inlet salt mass fraction for Cases SW3 and SW4 are presented in Figure 7.6. The mass fraction starts from the inlet value and increases by about 20% and 18% for Cases SW3 and SW4, respectively, as it approaches the channel outlet. This increase is a result of water mass transfer to the gas phase.

Figure 7.7 shows the effects changing the inlet salinity on the interfacial heat transfer for different wall heat flux values. The interface heat transfer increases with increasing wall heat flux. A greater amount of energy is added to the liquid as sensible heat for a higher wall heat flux, thereby

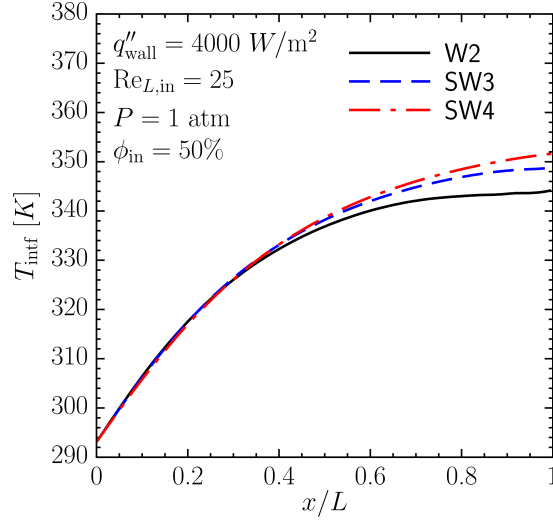


Figure 7.5: Temperature distribution at the interface along the channel

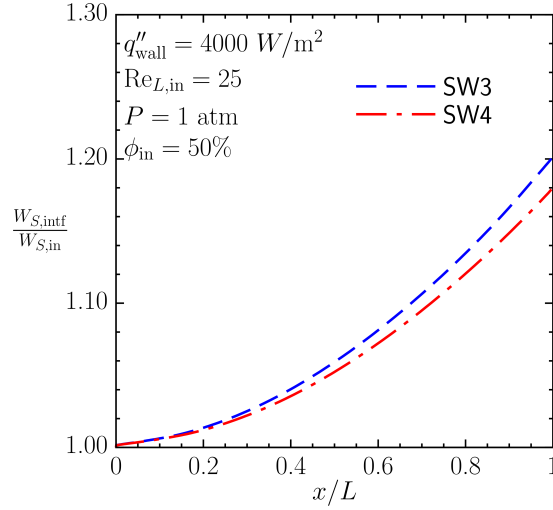


Figure 7.6: The interfacial salt mass fraction change along the channel

raising the temperature at the interface. Consequently, more heat and mass transfer occurs, leading to an increase in the evaporation rate. The interfacial heat flux decreases with salinity for both wall heat flux values. The primary reason behind the decrease in heat transfer at the interface is the elevation of the boiling point when increasing the inlet salt mass fraction. This implies that more energy is required to reach the boiling point for water evaporation. However, this decrease is not

substantial compared to other factors that impact heat transfer at the interface. For instance, the latent heat of vaporization decreases when the salt mass fraction increases in the liquid phase [107], meaning that less energy is required through the latent heat transfer process to achieve evaporation. Additionally, the specific heat of salt-water is lower than that of pure water, indicating that salt-water requires less energy for an equivalent temperature increase.

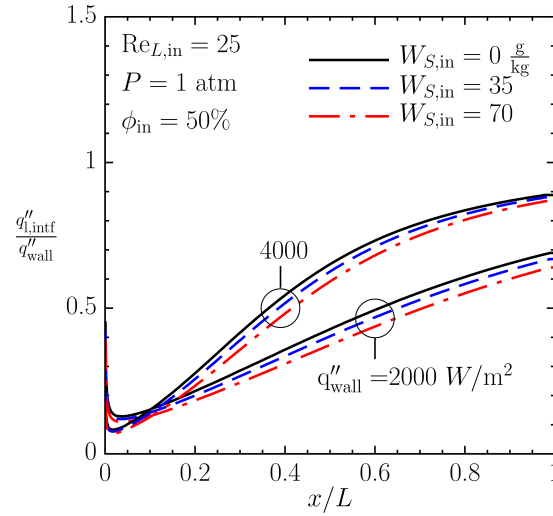


Figure 7.7: Interfacial heat flux change at the interface along the channel

The total relative amount of evaporated water per unit depth up to a given axially location, x , is defined as:

$$\dot{m}_{\text{tot},x}^{\star} = \frac{\sum_{x_i=0}^x \dot{m}'_{\text{inf}}(x_i)}{\dot{m}'_{L,\text{in}}(1 - W_s)} \quad (7.1)$$

Figure 7.8 depicts the axial variation of $\dot{m}_{\text{tot},x}^{\star}$ for the two different wall heat flux values. The total evaporated mass decreases with increasing the inlet salinity in the liquid phase. For a wall heat flux of 4000 W/m^2 , the total evaporated mass decreases by about 5% and 9.3% compared to the pure water case, for inlet salinities of 35 g/kg and 70 g/kg, respectively. The decrease in the total evaporated mass is related to the factors that affect interfacial heat transfer, as discussed earlier. The effect of salt mass fraction change on the total evaporated mass is the almost the same in both wall heat flux values. Comparing the pure water with the highest salinity test case, the total evaporated mass at the channel exit decreases about 12.9% and 9.3% for $q''_{\text{wall}} = 2000 \text{ W/m}^2$ and

$q''_{\text{wall}} = 4000 \text{ W/m}^2$, respectively.

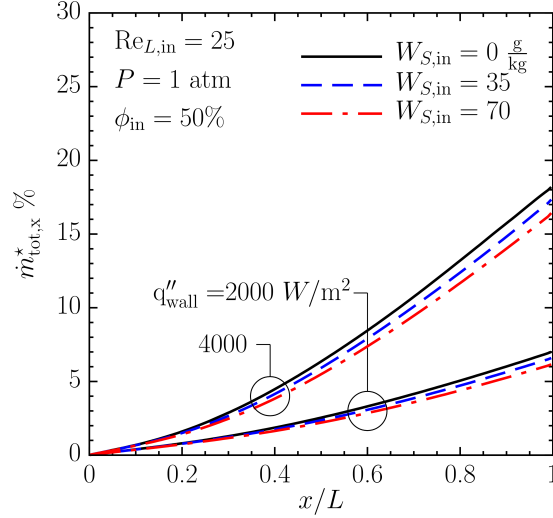


Figure 7.8: Total evaporated mass along the channel

The results were also examined using an effectiveness parameter, ϵ [32]. Figure 7.9 a shows the effectiveness for different $Re_{L,in}$, q''_{wall} , and $W_{S,in}$ values. The effectiveness increases by decreasing $Re_{L,in}$ due to a larger amount of energy available for the evaporation process. It increases 29.1% when $Re_{L,in}$ decreases from 35 to 25 at $q''_{\text{wall}} = 4000 \text{ W/m}^2$ and $W_{S,in} = 35 \text{ g/kg}$. The effectiveness is also improved for a higher wall heat flux because of the higher relative increase in evaporation rate. The effectiveness increases by 43.8% when q''_{wall} changes from 2000 to 4000 W/m^2 at $Re_{L,in} = 25$ and $W_{S,in} = 35 \text{ g/kg}$, which corresponds to a more than 100% increase of the total evaporation mass flow rate. Conversely, the effectiveness decreases with increasing the liquid salinity. For example, at $q''_{\text{wall}} = 4000 \text{ W/m}^2$ and $Re_{L,in} = 25$, the effectiveness is reduced by 5.4% and 10.5% as the inlet salinity changes from zero to 35 g/kg and 70 g/kg, respectively. The rate of change of effectiveness due to the salinity change is almost the same for other $Re_{L,in}$ and q''_{wall} values.

Desalination plants are mostly constructed close to the sea shores so that the seawater can be easily transported to the plant. Depending on the plant location and time of the year, the air relative humidity varies from 10% to 90%. Case SW3 was used to illustrate the impact of changing the relative humidity. For this case, the relative humidity varies in a range from 20% ($W_a = 0.997$)

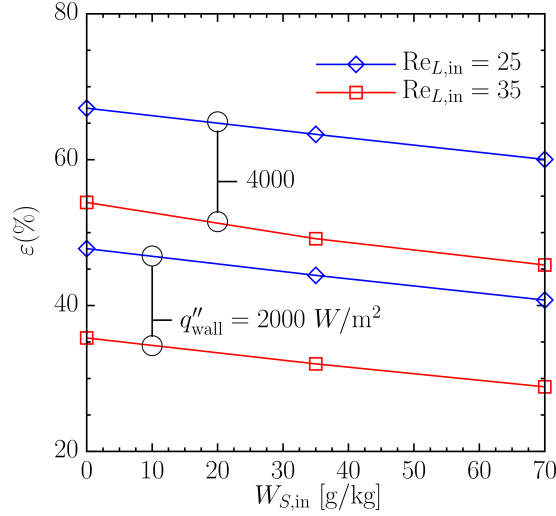


Figure 7.9: Effectiveness change with salt mass fraction for different inlet liquid Reynolds numbers and wall heat fluxes

to 80% ($W_a = 0.988$). Table 7.2 shows the maximum percent difference, Ψ , of interfacial field variables and $\dot{m}_{\text{tot},x}^*$ when the relative humidity changes from 50% to 20% or 80%. As is seen in this table, the maximum percent difference is not significant for any of the studied variables at the interface. The air relative humidity variation can change the inlet gas-vapour mixture properties, and based on the inlet fully-developed analytical solution, it affects the inlet liquid film thickness and consequently the inlet liquid and gas mass flow rates. However, this effect is not significant enough to noticeably change the inlet transport parameters. Therefore, the conclusion is that the change of relative humidity does not significantly influence the evaporation rate in the range of parameters studied here.

Table 7.2: Maximum percent difference of interfacial variables for different relative humidity values, in comparison with Case SW3 ($\phi = 50\%$)

ϕ	$\Psi(U)$	$\Psi(T)$	$\Psi(W_s)$	$\Psi(W_a)$	$\Psi(\dot{m}_{\text{tot},x}^*)$
20%	0.33	0.14	0.004	0.23	0.05
80%	0.30	0.12	0.004	0.55	0.17

Chapter 8

Desalination Process on Horizontal Tubes: Elliptic Model

8.1 Introduction

In this chapter, the previously developed in-house code is utilized to simulate the evaporation from falling films of fresh water and salt water over horizontal tubes. The elliptic solution approach, which is capable of capturing the reverse flow and recirculation zones, is used for the simulations. The accuracy of the model is verified by comparing the present results with relevant experimental and numerical data available in the literature. The results from the present two-phase elliptic model are compared with the experimental data presented by Chen et al. [2], Hu and Jacobi [4], and Shen et al. [5] and two-phase numerical model developed by Wang et al. [3]. New numerical results are provided for a parametric study examining how variations in inlet salt mass fraction, inlet pressure, inlet mixture Reynolds number, wall temperature, and inlet liquid mass flow rate affect the falling film development, heat transfer, and evaporation rate around the tube.

8.2 Grid Independence Study

A study was conducted to assess the grid independence of the results for a selected grid. A case with $P_{\text{in}} = 1$ atm, $\text{Re}_{M,\text{in}} = 50$, $\dot{m}''_{L,\text{in}} = 0.022 \frac{\text{kg}}{\text{m}^2\text{s}}$, and $S_{\text{in}} = 35$ g/kg was chosen for testing with various grid resolutions. Number of grids in the domain, N_x , $N_{y,L}$, and $N_{y,G}$, defined in Chapter 3, were adjusted to determine their impact on the flow parameters. Different grid configurations were utilized, ranging from 160 to 580, 15 to 60, and 35 to 145 for N_x , $N_{y,L}$, and $N_{y,G}$, respectively. Compared to the finest grid ($N_x = 580$, $N_{y,L} = 60$, and $N_{y,G} = 145$), a grid with $N_x = 390$, $N_{y,L} = 30$,

and $N_{y,G} = 105$ showed reasonable maximum percent differences in the angular profiles for different variables listed in Table 8.1. Because the differences are not significant, the aforementioned grid was used in all simulations for the present study.

Table 8.1: Deviations between angular profiles for the selected grid and the finest grid for key quantities

Variable	Maximum percent difference (%)
δ	0.17
U_{intf}	1.58
T_{intf}	0.02
$W_{s,\text{intf}}$	0.003
$W_{g,\text{intf}}$	0.04

8.3 Comparisons with Previous Work

8.3.1 Definition of Comparison Cases

In this section, the in-house code developed in this work has been validated against previous experimental and numerical studies. Film thickness is compared with experimental data from Chen et al. [2] and numerical results from Wang et al. [3] under adiabatic condition for pure water and salt water, respectively. Additionally, the local heat transfer coefficient is compared with experimental studies conducted by Hu and Jacobi [4] and Shen et al. [5], under uniform wall heat flux condition for pure and salt water, respectively. The geometric and operating parameters used in comparison cases are summarized in Table 8.2. A tube bundle and the geometric parameters defined for horizontal tubes are depicted in Figure 8.1. L_2 is set to $5D$ for all cases. The grid resolution is the same as the one selected in Section 8.2, with some adjustments made to the grid axial expansion ratio. In the studies referenced, either the liquid mass flow rate or the liquid Reynolds number is reported.

8.3.2 Inlet film thickness calculation

Depending on the experimental setup, the distance between the inlet and the tube surface at $\theta = 0^\circ$ (L_0) could be different. A greater distance results in a thinner film thickness and a higher local heat transfer coefficient around the tube. Thus, L_0 is considered a key parameter for improving heat and mass transfer in the system; however, an excessively high distance can cause a discontinuous film, which negatively affects system performance. In order to keep the computational domain size reasonable, the distance L_1 , which is depicted in Figure 8.1 could be adjusted in the numerical simulations by specifying the velocity and film thickness at the inlet. In an experimental setup, the inlet velocity is assumed to be equal to the free-fall velocity from the upper tube [108]:

$$U_{L,\text{in}} = \sqrt{2g(L_0 - L_1)} \quad (8.1)$$

L_1 is set to $0.5D$ in the first three cases listed in the table and is set to $0.77D$ for Case SW2. Therefore, the distance $(L_0 - L_1)$ is calculated based on a desired entry length L_1 in the computational domain and L_0 defined in the experimental study. The inlet velocity is then calculated using Equation (8.1). The inlet film thickness, δ_{in} , is subsequently calculated based on the specified inlet liquid mass flow rate per unit depth.

$$\delta_{\text{in}} = \frac{\dot{m}'_{L,\text{in}}}{\rho_L U_{L,\text{in}}} \quad (8.2)$$

Table 8.2: Geometric and operating parameters in comparison cases.

Reference	Case	D	$\dot{m}'_{L,\text{in}}$	$\text{Re}_{L,\text{in}}$	$\text{Fr}_{L,\text{in}}$	δ_{in}	P	q''_{wall}	$T_{L,\text{in}}$	$T_{G,\text{in}}$	$W_{s,\text{in}}$	Gas	ψ_{in}
		[mm]	[kg m ⁻¹ s ⁻¹]	—	—	[mm]	[kPa]	kW m ⁻²	[°C]	[°C]	—	phase	(%)
Chen et al. [2]	PW1	25.4	—	184	213	0.15	101.33	0	20	20	0	AVM	50
Wang et al. [3]	SW1	25.4	—	258	309.6	0.15	101.33	0	20	20	0.03	AVM	50
Hu and Jacobi [4]	PW2	22	—	245	4.91	1	101.33	15	30	20	0	AVM	50
Shen et al. [5]	SW2	19	0.026	—	42	0.25	12.35	7.75	50	50	0.03	PV	0

AVM: Air-Vapour Mixture; PV: Pure Vapour

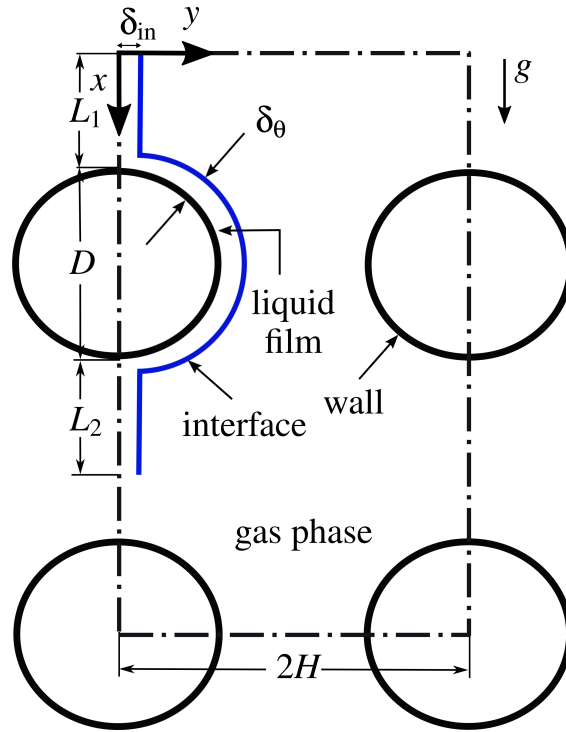


Figure 8.1: Geometric parameters defined for horizontal tubes.

8.3.3 Comparison of the Film Thickness

Figure 8.2 (a) demonstrates the variation in water falling film thickness along the circumferential angle, compared with Case PW1. The results show a maximum percent difference of 11.03 at the circumferential location of 30° . This indicates a very good agreement between the present results and the measurements. Figure 8.2 (b) depicts the salt water falling film thickness compared with Case SW1. Again, the film characteristics show good agreement with previous numerical results. The maximum percent difference is 25.02, observed at the circumferential location of 165° .

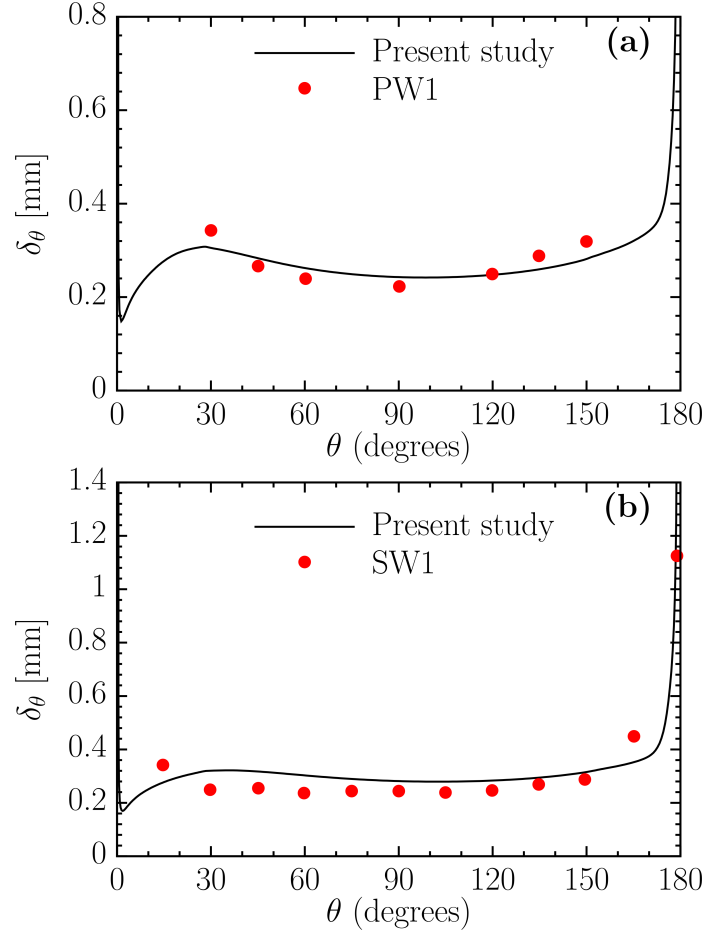


Figure 8.2: Comparison of the film thickness variation around the tube for (a) Case PW1 with experimental data [2], and (b) Case SW1 with numerical results [3].

8.3.4 Comparison of the Local Heat Transfer Coefficient

The local heat transfer coefficient around the tube is calculated using:

$$h_\theta = \frac{q''_{\text{wall}}}{T_{\text{wall}} - T_{L,\text{in}}} \quad (8.3)$$

Figure 8.3 shows the heat transfer coefficient around the tube compared with Case PW2 and Case SW2 for pure and salt water falling films, respectively. As seen in the figure, the heat transfer coefficient is over-predicted at the upper stagnation point for both cases. However, the trend

predicted by the code is consistent with the experimental data. Because q''_{wall} and $T_{L,\text{in}}$ are fixed in these cases, the discrepancy at the top of the tube must be related to the under-prediction of T_{wall} at that region. Figure 8.4 depicts the variation of wall temperature around the tube for Case PW2. As shown in this figure, the wall temperature is close to the inlet temperature when reaching the tube surface. Because the velocity is high, there is no opportunity for the film to heat up quickly at that region, and therefore the wall temperature at the top of the tube remains low. The wall temperature then increases with a sharp gradient over the tube up to an angular position of 60° , and beyond that, the increase rate becomes smoother. A sharp decrease of the wall temperature is observed at the bottom of the tube which is due to the creation of a recirculation zone at that region. A similar wall temperature spike was observed for Case SW2 at the top of the tube. In the experimental setup, the wall temperature could be affected by the axial conduction in the tube wall caused the temperature to be more uniform than that predicted by the numerical simulation at the top of the tube. For other regions, the results align well with the measurements, and the maximum percent differences are 18.3 and 16.2 for Case PW2 and Case SW2, respectively.

8.4 New Results for the Elliptic Two-phase Evaporation over a Horizontal Tube

In this section, flow hydrodynamics and heat and mass transfer of salt water falling film in the vicinity of a co-current gas flow are investigated. The liquid film is exposed to an isothermal tube surface. The inlet salinity ranges from 0 to 70 g/kg. The inlet pressure is adjusted to achieve an inlet saturation temperature ranging from 60 to 100 °C. In cases where only pure vapour is present in the gas phase ($P_{\text{in}} = 19.9$ kPa corresponding to a saturation temperature of 60 °C), the pure water liquid film is saturated, and the salt water liquid film is slightly sub-cooled. For cases where the gas phase consists of a mixture of vapour and air, the liquid falling film is sub-cooled. The relative humidity is set to 50% which corresponds to an air mass fraction of 0.86 and 0.94

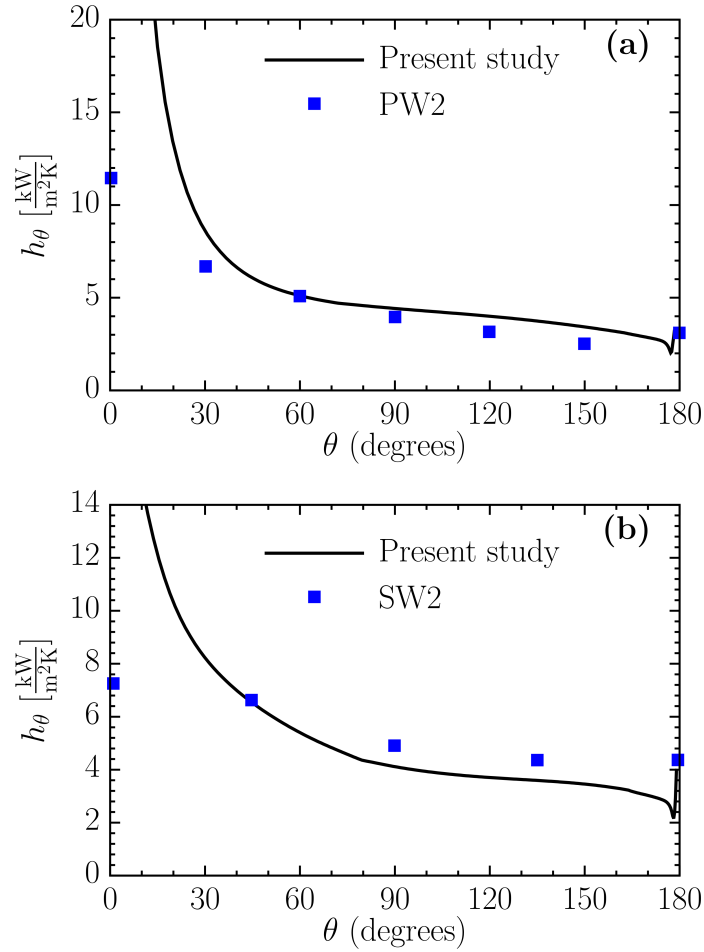


Figure 8.3: Comparison of the local heat transfer coefficient variation around the tube for (a) Case PW2 with experimental data [4], and (b) Case SW2 with experimental data [5].

for inlet pressures of 47.39 and 101.33 kPa, respectively. The inlet liquid mass flow rate per unit depth is either 0.022 or 0.033 $\frac{\text{kg}}{\text{m}\cdot\text{s}}$, which corresponds to the inlet liquid Reynolds number ranging from 158 to 284 for different amounts of salinity at the inlet. The mixture Reynolds number varies between 25 to 100. T_{wall} is either 60 or 70 °C. Other variables common to all simulations are: $T_{L,\text{in}} = 60$ °C, $T_{M,\text{in}} = 60$ °C, $\delta_{\text{in}} = 1$ mm, $D = 14$ mm, $L_1 = D/2$, $L_2 = 5D$, and $H = 5D$. Based on a study by Mitrovic [109], when the difference between the wall and evaporation temperatures is less than a certain value, nucleate boiling does not occur in the system. This temperature difference is a

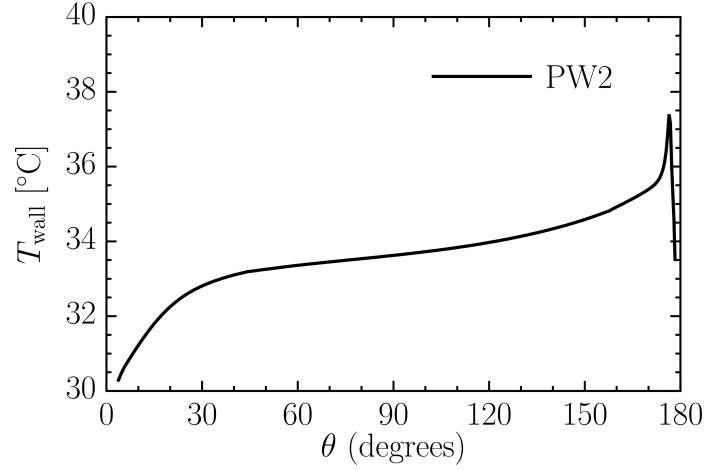


Figure 8.4: Wall temperature variation around the tube for Case PW2.

critical parameter because nucleate boiling can lead to a dry surface and deteriorate the evaporation and heat transfer in the system. Mitrovic reported that, for evaporation temperatures of 365 K and 315 K, the temperature differences could be about 3 K and 14 K, respectively, within the inlet liquid Reynolds number range specified in the present study. Therefore, as the temperature difference between the tube surface and liquid film does not exceed 10 K in the present study, it is assumed that for cases where the inlet liquid film is saturated, no nucleate boiling occurs within the falling film, and the liquid film only evaporates at the liquid-gas interface.

8.4.1 Effects of P_{in} , $Re_{M,in}$, T_{wall} and $\dot{m}'_{L,in}$ Variation on the Flow Hydrodynamics

To investigate the effects of changing the inlet pressure, mixture Reynolds number, wall temperature, and liquid mass flow rate on the flow characteristics and liquid film thickness, several selected cases with a salinity of 35 g/kg were studied.

Figure 8.5 (a) shows the flow streamlines for a case with $P_{in} = 19.9$ kPa and $Re_{M,in} = 25$. The x and y axes are scaled by dividing their values by the total length ($L_1 + D + L_2$) and width (H)

of the domain, respectively. The liquid in the vicinity of a co-current gas flow enters the system with a uniform velocity profile. The velocity gradually increases due to gravity until it reaches the tube surface. When the film hits the tube surface, it suddenly decelerates at the upper stagnation point. It then flows over the tube surface, where its temperature increases due to heat transfer from the wall to the liquid. The film velocity decreases again at the lower stagnation point and finally detaches from the surface. The flow in the gas phase could be affected by buoyancy forces. In this case, only pure vapour is present in the gas phase; therefore, there is no solutal buoyancy influencing the flow pattern. Thermal buoyancy acts as an opposing force in the system; however, in this case, it is not strong enough to affect the co-current gas flow. Consequently, the gas flow eventually exits the system at the outlet boundary. Figure 8.5 (b) depicts flow streamlines for a case at the atmospheric pressure ($P_{in} = 101.33$ kPa) where an air-vapour mixture is present in the gas phase and $Re_{M,in} = 25$. Although the flow characteristics around the tube are similar to those at the lower inlet pressure, flow reversal is observed at the outlet boundary, and it affects the flow upstream up to $X = 0.4$. In the case that reversal flow occurs, a special treatment for outlet boundary conditions is needed, as mentioned in Chapter 2. This reversal is thought to be due to the dominance of upward buoyancy forces over other forces in the gas flow direction. In this case, both thermal and solutal buoyancy forces are present in the system. The occurrence of flow reversal at the outlet mainly depends on the mixture Reynolds number, the air mass fraction, and wall temperature in the system. Figure 8.5 (c) shows the flow streamlines for a case with $P_{in} = 101.33$ kPa and $Re_{M,in} = 50$. As shown in this figure, the outlet boundary is still affected by the dominance of buoyancy forces; however, due to a stronger forced convection, it only impacts a small area close to the exit boundary.

Before the film detaches from the surface, a recirculation zone forms at the lower stagnation point, which could affect heat transfer in that region. Figure 8.6 illustrates the recirculation zones observed for $P_{in} = 19.9$ kPa and $P_{in} = 101.33$ kPa, respectively. The recirculation zones are similar in size and centre location.

To measure the strength of the buoyancy forces, two Grashof numbers are defined for the

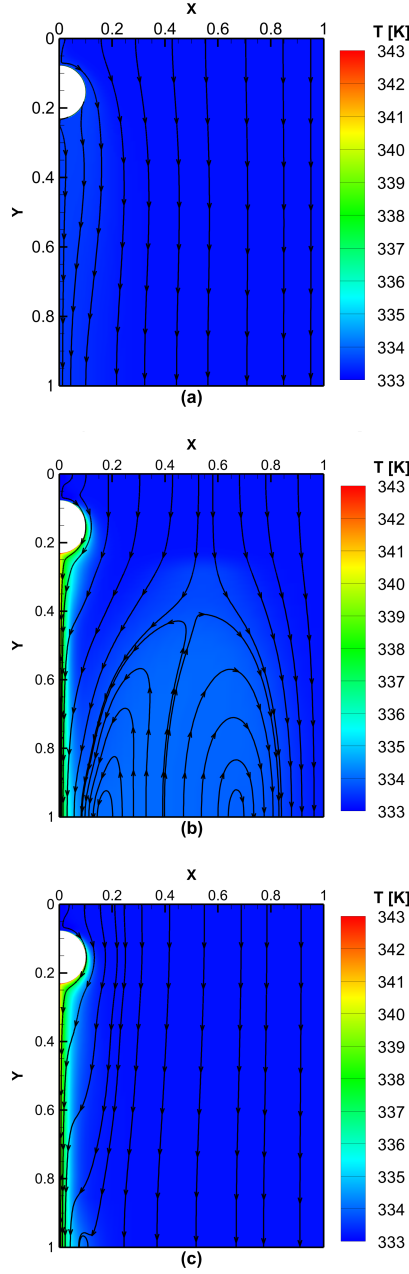


Figure 8.5: Flow streamlines for cases with $\dot{m}'_{L,in} = 0.022 \frac{\text{kg}}{\text{m}\cdot\text{s}}$, $T_{\text{wall}} = 70 \text{ }^{\circ}\text{C}$ (343.15 K), and (a) $P_{\text{in}} = 19.9 \text{ kPa}$ and $\text{Re}_{M,in} = 25$, (b) $P_{\text{in}} = 101.3 \text{ kPa}$ and $\text{Re}_{M,in} = 25$, and (c) $P_{\text{in}} = 101.3 \text{ kPa}$ and $\text{Re}_{M,in} = 50$.

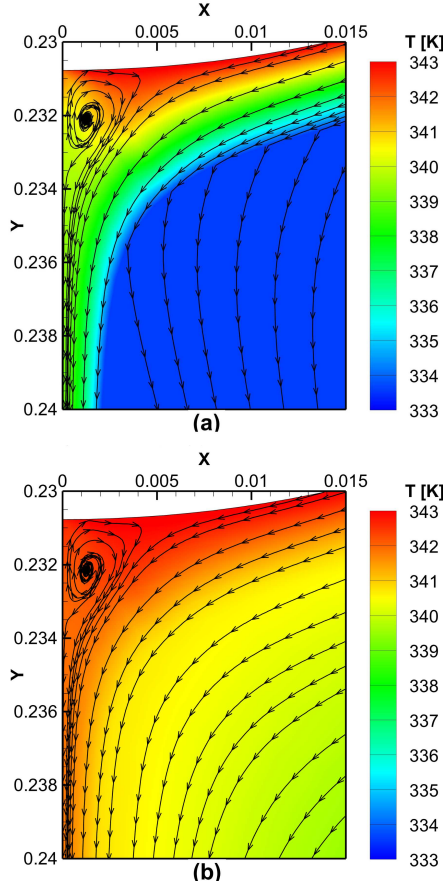


Figure 8.6: Recirculation zones observed in the liquid film for cases with $\dot{m}'_{L,in} = 0.022 \frac{\text{kg}}{\text{m}\cdot\text{s}}$, $\text{Re}_{M,in} = 25$, $T_{\text{wall}} = 70 \text{ }^\circ\text{C}$ (343.15 K), and (a) $P_{\text{in}} = 19.9 \text{ kPa}$ and (b) $P_{\text{in}} = 101.3 \text{ kPa}$.

horizontal tubes:

$$\text{Gr}_T = \frac{g (T_{\text{intf}} - T_{M,\text{in}}) D^3}{\nu_M^2 T_{M,\text{in}}} \quad (8.4)$$

$$\text{Gr}_M = \frac{g (M_a/M_v - 1) (W_{a,\text{in}} - W_{a,\text{intf}}) D^3}{\nu_M^2} \quad (8.5)$$

where Gr_T and Gr_M are the thermal and mass Grashof numbers, respectively.

The average Grashof numbers are also defined as:

$$\overline{\text{Gr}}_T = \frac{2}{\pi D} \int_0^{\frac{\pi D}{2}} \text{Gr}_T dx \quad (8.6)$$

$$\overline{\text{Gr}}_M = \frac{2}{\pi D} \int_0^{\frac{\pi D}{2}} \text{Gr}_M dx \quad (8.7)$$

Figure 8.7 shows the variation of the thermal Grashof number with the circumferential angle for $P_{\text{in}} = 19.9$ kPa, $P_{\text{in}} = 47.4$ kPa, and $P_{\text{in}} = 101.3$ kPa, and mass Grashof number variation with the circumferential angle for $P_{\text{in}} = 47.4$ kPa and $P_{\text{in}} = 101.3$ kPa. The cases with a higher inlet pressure are affected not only by a higher thermal Grashof number but also by a significant mass Grashof number. For higher inlet pressure cases where air is present in the gas stream, the thermal Grashof number is negative in the upper part of the tube. This trend is due to a lower interface temperature compared to the inlet temperature in that region. In the upper part of the tube, the concentration difference between the liquid and gas phases leads to the evaporation of some liquid, accompanied by heat transfer from the falling film to the gas flow. Additionally, because the falling film has just come into contact with the wall, it has not yet been significantly affected by the surface temperature. As a result, a slight drop in the interface temperature is observed at the top of the tube. Because the interface temperature and air mass fraction are increasing, both Grashof numbers increase along the tube surface. At $P_{\text{in}} = 19.9$ kPa, however, the change of thermal Grashof number is not noticeable, indicating negligible variation of the interface temperature along the tube surface.

Tables 8.3 and 8.4 list the average Grashof numbers for different variable combinations. The buoyancy forces are more noticeable for the higher P_{in} (higher air mass fraction) due to increased density, which, at a constant $\text{Re}_{M,\text{in}}$, reduces the velocity in the gas phase. Additionally, at a constant inlet pressure, the effects of buoyancy forces are more pronounced for a lower $\text{Re}_{M,\text{in}}$ because of smaller downward flow resistance against upward buoyancy forces due to a lower velocity in the gas phase. An increase in wall temperature raises both Grashof numbers. The thermal Grashof number increases due to a higher amount of heat transferred to the liquid film, and the mass Grashof number increases due to a higher rate of evaporation and air replacement with vapour at the interface. The effects of buoyancy forces are also more pronounced for lower $\dot{m}'_{L,\text{in}}$, which is expected to be due to a higher evaporation rate at a lower inlet mass flow rate. The cases in which flow reversal occurs are indicated in the tables. Flow reversal is observed for higher inlet pressures,

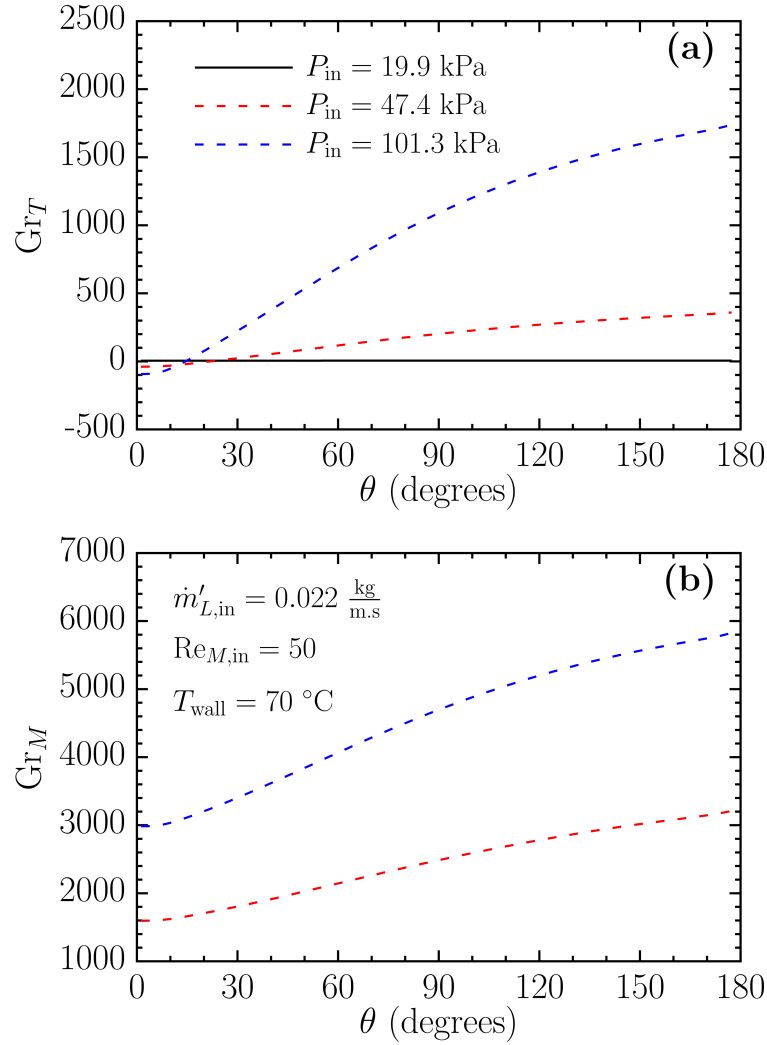


Figure 8.7: Local Grashof numbers for different inlet pressures (a) thermal Grashof number, (b) mass Grashof number.

lower mixture Reynolds numbers, and higher wall temperature, which may lead to the dominance of opposing buoyancy forces over convective forces in the system.

Figure 8.8 shows the variation in film thickness over the tube surface for different inlet pressures, mixture Reynolds numbers, wall temperatures, and liquid mass flow rates. Film thickness

Table 8.3: Grashof numbers for parametric study cases ($\dot{m}'_{L,in} = 0.022 \frac{\text{kg}}{\text{m}\cdot\text{s}}$).

	$\text{Re}_{M,in}$ –	T_{wall} [°C]	$P_{\text{in}} = 19.9$ [kPa]	$P_{\text{in}} = 47.4$ [kPa]	$P_{\text{in}} = 101.3$ [kPa]
Gr_T	25	65	5.17	75.08 *	439.92 *
		70	5.38	192.39 *	984.43 *
	50	65	5.15	65.93	426.85
		70	5.38	181.97	970.07 *
	100	65	5.15	56.37	408.8
		70	5.37	171.05	949.17
Gr_M	25	65	–	2000.48	3724.08
		70	–	2485.84	4585.81
	50	65	–	1966.41	3705.00
		70	–	2440.63	4561.89
	100	65	–	1931.86	3678.88
		70	–	2395.42	4527.58

* Cases with flow reversal at the outlet

Table 8.4: Grashof numbers for parametric study cases ($\dot{m}'_{L,in} = 0.033 \frac{\text{kg}}{\text{m}\cdot\text{s}}$).

	$\text{Re}_{M,in}$	T_{wall} [°C]	$P_{\text{in}} = 19.9$ [kPa]	$P_{\text{in}} = 47.4$ [kPa]	$P_{\text{in}} = 101.3$ [kPa]
Gr_T	25	65	5.07	30.62 *	237.64 *
		70	5.22	105.53 *	581.16 *
	50	65	5.07	24.67	228.66
		70	5.22	98.35	572.16 *
	100	65	5.07	16.47	214.07
		70	5.22	89.74	555.92
Gr_M	25	65	–	1836.21	3432.92
		70	–	2122.00	3941.60
	50	65	–	1815.28	3420.41
		70	–	2094.07	3928.01
	100	65	–	1786.86	3400.17
		70	–	2061.68	3903.55

* Cases with flow reversal at the outlet

is defined as the normal distance between the tube surface and the liquid-gas interface, so it approaches infinity at the top and bottom of the tube, where θ equals 0° and 180° , respectively. The normalized film thickness is only depicted up to $\delta_\theta/\delta_{in} = 0.35$ in this figure, in order to focus on the variation over the tube. As the liquid film reaches the tube surface, it becomes thinner over a specific section (up to 3°) before quickly thickening as it flows over the tube surface. After reaching its maximum value due to the liquid accumulation in the impingement region, at a circumferential angle of less than 30° , the film thickness decreases until it reaches a minimum value after 90° . This decrease is due to the increase of the vertical gravity component along the circumferential angle. After that, the film slightly thickens under the impact of shrinking vertical gravity component. The vortex created in the lower part of the tube causes a sharp increase of the film thickness while detaching from the surface and then approaches infinity at 180° .

As illustrated in this figure, film thickness is not significantly affected by the inlet pressure or mixture Reynolds number. The film thickness slightly thins by increasing $Re_{M,in}$ and reducing P_{in} at the upper half part of the tube. It decreases with rising wall temperature because a higher wall temperature facilitates the evaporation of the falling film and mass transfer to the gas phase. Film thickness also increases with rising inlet liquid mass flow rate, which is due to a higher inlet velocity and stronger flow acceleration after the impingement region at the top of the tube. Predicting the minimum film thickness is crucial as it determines the maximum acceptable inlet liquid mass flow rate to prevent a dry surface. The location of the minimum film thickness shifts from 99.5° to 105.4° as the mass flow rate increases from 0.022 to $0.033 \frac{\text{kg}}{\text{m}\cdot\text{s}}$.

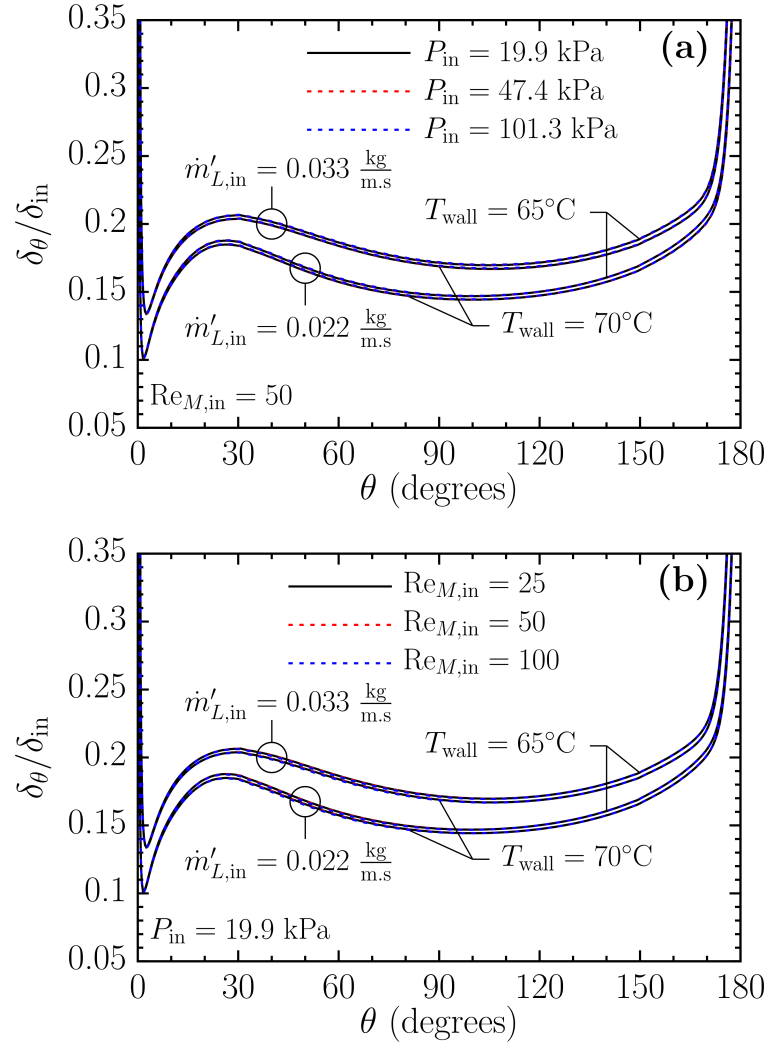


Figure 8.8: Liquid film thickness variation around the tube for different amounts of P_{in} , $Re_{M,in}$, $m'_{L,in}$, and T_{wall} .

8.4.2 Effects of P_{in} Variation on the Heat and Mass Transfer

Figure 8.9 depicts the variation of interface temperature around the tube. When $P_{in} = 19.9$ kPa, the interface temperature is nearly constant and similar to the inlet temperature for both wall temperature values, indicating that the vapor pressure does not change significantly at the interface. This trend results in a constant saturation temperature at the interface. For the two other pressures, the interface temperature increases around the tube. The interface temperature is lower than the inlet temperature up to a circumferential angle of approximately 30° . This decrease is due to a relatively high rate of heat and mass transfer to the gas phase while the falling film has not been significantly impacted by the temperature difference between the wall and the liquid film, which consequently lowers the interface temperature. However, the temperature increases after 30° due to the heat added to the film and an increase in vapor partial pressure and mass fraction at the interface. For $T_{wall} = 70^\circ\text{C}$, the interface temperature increase is more noticeable compared to the case of $T_{wall} = 65^\circ\text{C}$. For $P_{in} = 101.3$ kPa, the interface temperature increases about 6.2% at the bottom of the tube when the wall temperature increases from 65°C to 70°C . Additionally, when $T_{wall} = 65^\circ\text{C}$, the interface temperature is up to about 1 K higher for $P_{in} = 101.3$ kPa compared to $P_{in} = 47.4$ kPa. As seen in Figure 8.9 (b), the temperature increase around the tube is more pronounced for a lower inlet mass flow rate. For $P_{in} = 101.3$ kPa, the interface temperature at the bottom of the tube increased about 2 K when the inlet liquid mass flow rate decreased from 0.033 to $0.022 \frac{\text{kg}}{\text{m}\cdot\text{s}}$.

Figure 8.10 demonstrates the local heat transfer changes around the tube. The maximum heat transfer coefficient is observed at the top of the tube (up to a circumferential angle of 10°) due to the liquid impingement at that location. The heat transfer coefficient then rapidly decreases in the developing region (from 10° to 30°), where most of the energy from the wall is used to increase the film temperature. This decrease continues at a more gradual rate because of a reduction in the temperature gradient close to the wall. The coefficient increases in the departure region (a circumferential angle more than 175°) due to the formation of a vortex at the bottom of the tube.

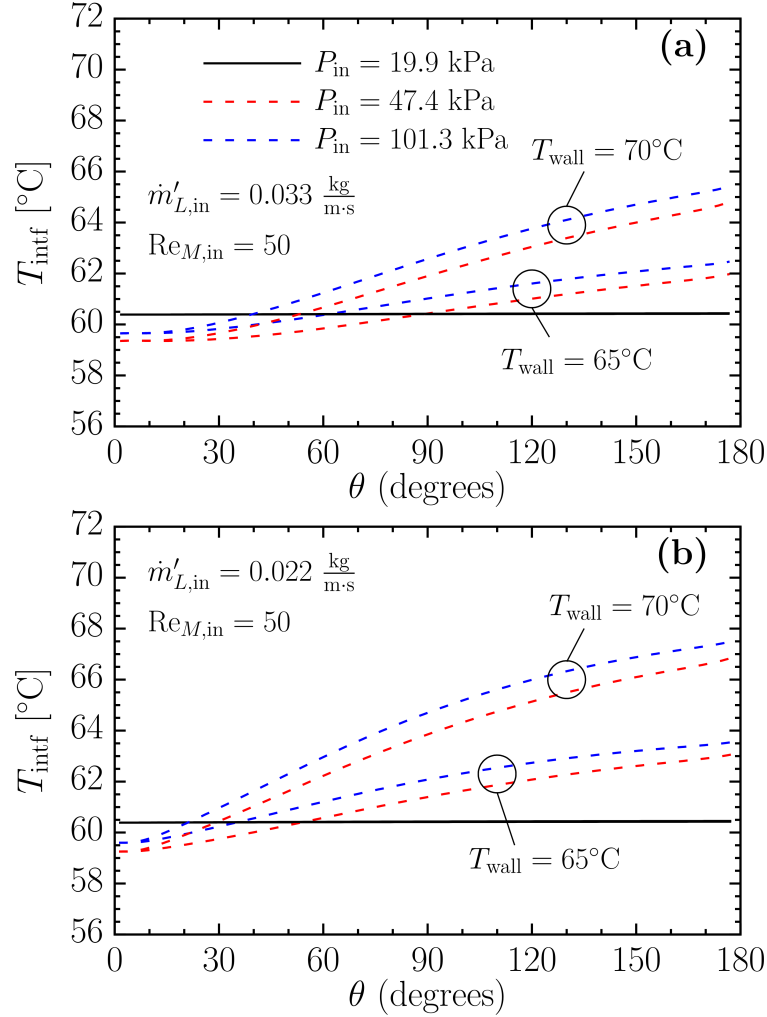


Figure 8.9: Interface temperature variation around the tube for different amounts of P_{in} , $\dot{m}'_{L,\text{in}}$, and T_{wall} .

It is important to note that the decrease in film thickness reduces the conduction resistance in the falling film. However, the heat transfer coefficient does not increase similarly with the decreasing conduction resistance, indicating that convection effects play a more significant role in the system. Figure 8.10 (a) shows the variation of h_θ around the tube at $P_{\text{in}} = 19.9$ kPa for two inlet liquid mass flow rate values. The variation of h_θ is smooth from 30° to 150° , reflecting a small temperature gradient close to the wall in that region. An increase in the inlet mass flow rate increases h_θ up to

a circumferential angle of 60° , after which h_θ decreases with increasing inlet mass flow rate. As discussed earlier, film thickness increases with the increase of the inlet liquid mass flow rate. From 30° to 60° , convection effects dominate due to a higher velocity, while a thicker liquid film leads to stronger conduction resistance beyond 60° , resulting in a reduction in h_θ . For other inlet pressure cases, h_θ increases with increasing $\dot{m}'_{L,in}$, indicating that the impact of convection on h_θ is more noticeable than the increase in film thickness. Additionally, for higher pressures, the decrease in h_θ around the tube occurs at a higher rate due to a larger temperature difference in the liquid film.

The effects of inlet pressure changes on the total evaporated mass are shown in Figure 8.11. As seen in this figure, the evaporation rate increases substantially for the case with $P_{in} = 19.9$ kPa, which is for pure vapour. These results indicate that the presence of air in the gas phase negatively affects the mass transfer and evaporation process. Additionally, in subcooled cases, a significant amount of energy is used to raise the film temperature rather than increasing the latent heat transfer and evaporation rate. For $\dot{m}'_{L,in} = 0.033 \frac{\text{kg}}{\text{m}\cdot\text{s}}$ and $T_{wall} = 65^\circ\text{C}$, the total evaporated mass increases by about five times when the inlet pressure decreases from $P_{in} = 101.3$ kPa to $P_{in} = 19.9$ kPa. The total evaporated mass increases with an increase in wall temperature due to a higher amount of energy added to the falling film, which facilitates the liquid evaporation into the gas phase. When $\dot{m}'_{L,in} = 0.033 \frac{\text{kg}}{\text{m}\cdot\text{s}}$ and $P_{in} = 19.9$ kPa, the rise in wall temperature doubles the total evaporation rate. The total evaporated mass decreases for a higher $\dot{m}'_{L,in}$, which is consistent with the results presented by Louahlia-Gualous and Omari [110]. This could be due to a longer residence time of the liquid in contact with the tube surface. By decreasing the liquid mass flow rate, the energy required to heat the liquid film also decreases. Additionally, the amount of advected energy to the downstream is reduced, which could enhance the latent heat transfer and the evaporation rate. For $P_{in} = 19.9$ kPa and $T_{wall} = 65^\circ\text{C}$, the total evaporated mass increases by about 40% when decreasing $\dot{m}'_{L,in}$ from 0.033 to $0.022 \frac{\text{kg}}{\text{m}\cdot\text{s}}$.

Figure 8.12 shows the change in interface salt mass fraction around the tube. The interface salt mass fraction increases around the tube for all pressures; however, the increase is more pronounced at the lowest inlet pressure. When $\dot{m}'_{L,in} = 0.022 \frac{\text{kg}}{\text{m}\cdot\text{s}}$ and $T_{wall} = 70^\circ\text{C}$, the amount of salt at the

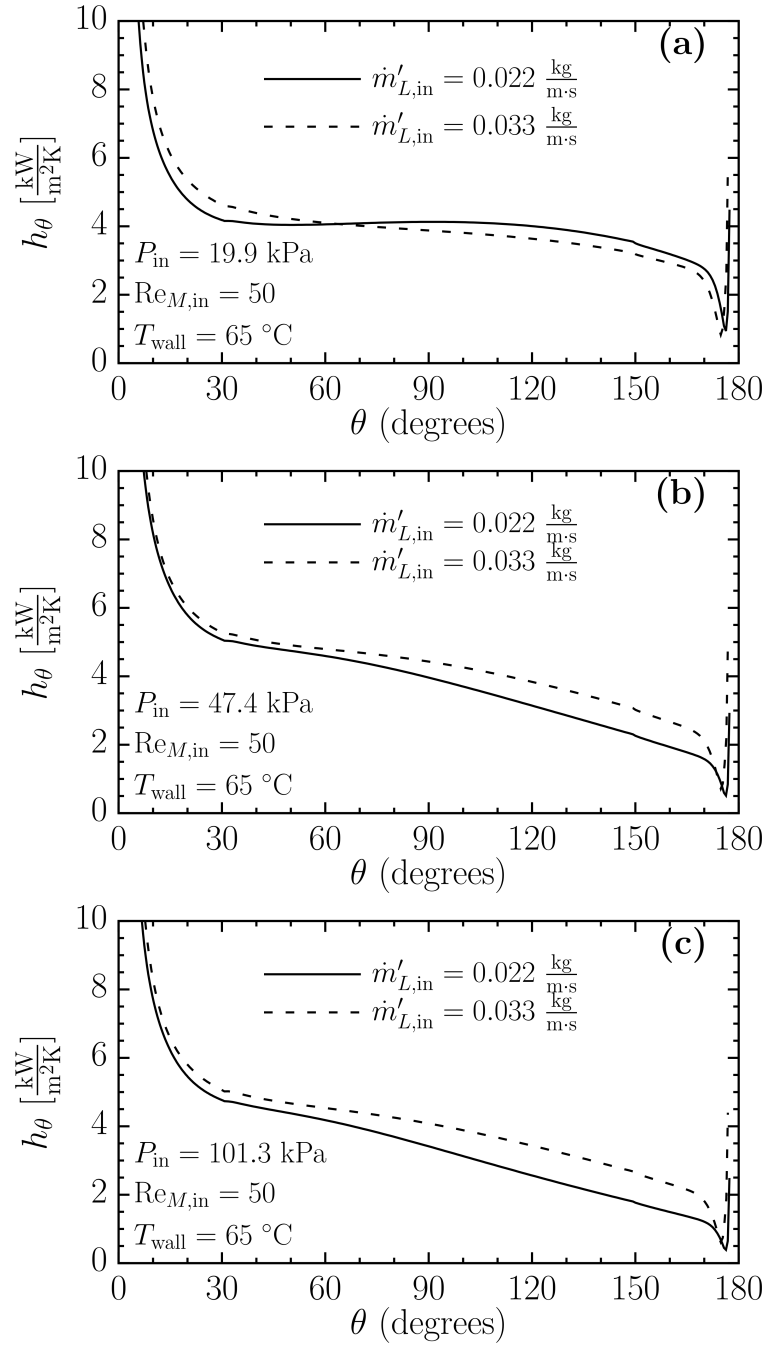


Figure 8.10: Local heat transfer coefficient variation around the tube for different amounts of P_{in} and $\dot{m}'_{L,\text{in}}$.

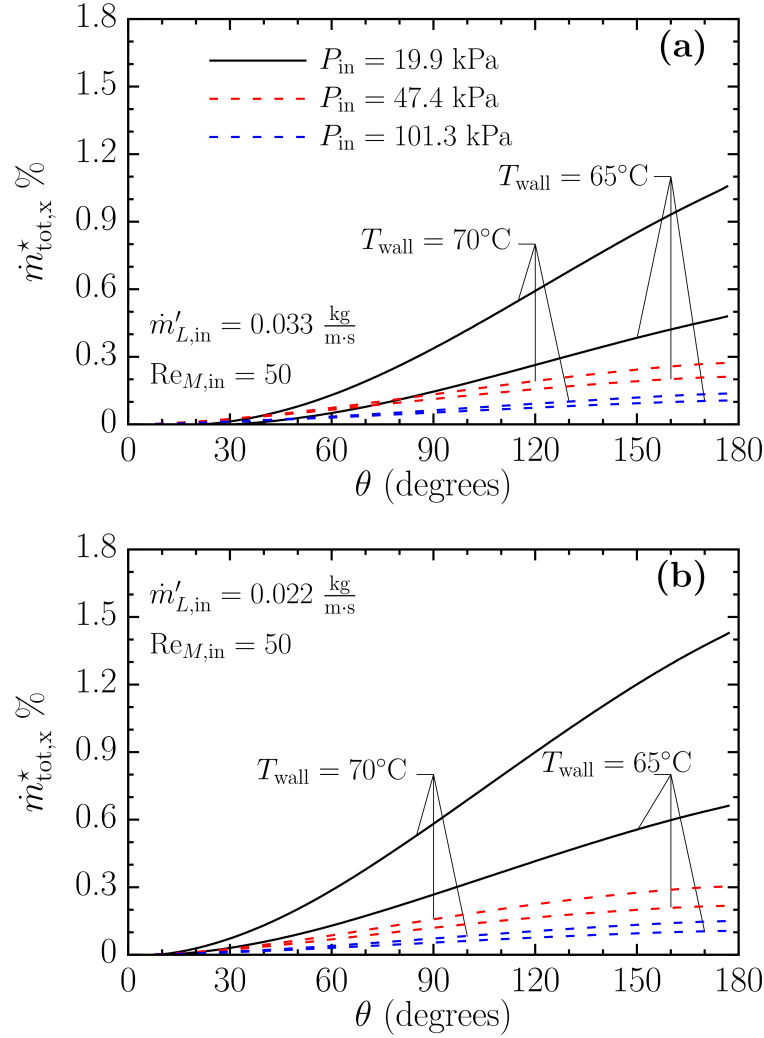


Figure 8.11: Total evaporated mass around the tube for different amounts of P_{in} , $\dot{m}'_{L,in}$, and T_{wall} .

bottom of the tube is approximately 6.5% higher for $P_{in} = 19.9$ kPa compared to $P_{in} = 101.3$ kPa. Additionally, an increase in wall temperature leads to a higher salt concentration at the interface. For $\dot{m}'_{L,in} = 0.022 \frac{\text{kg}}{\text{m}\cdot\text{s}}$ and $P_{in} = 19.9$ kPa, the interface salt mass fraction increases about 4.2% when increasing the wall temperature from 65°C to 70°C . The increase in salt mass fraction at the interface is directly related to a higher evaporation rate as the high evaporation rate results in salt accumulation at the interface. When the falling film reaches the tube surface, the interface salt mass fraction is less than that of the inlet at $P_{in} = 19.9$ kPa, but higher than the inlet mass fraction

at the other two pressures. For $P_{in} = 19.9$ kPa, it is due to condensation of some vapour into the liquid film. For $P_{in} = 47.4$ kPa and $P_{in} = 101.3$ kPa, the higher interface mass fraction is due to the evaporation of a small amount of liquid into the gas phase in the region above the tube because of the concentration difference at the interface. However, these amounts are negligible and do not significantly affect the overall process.

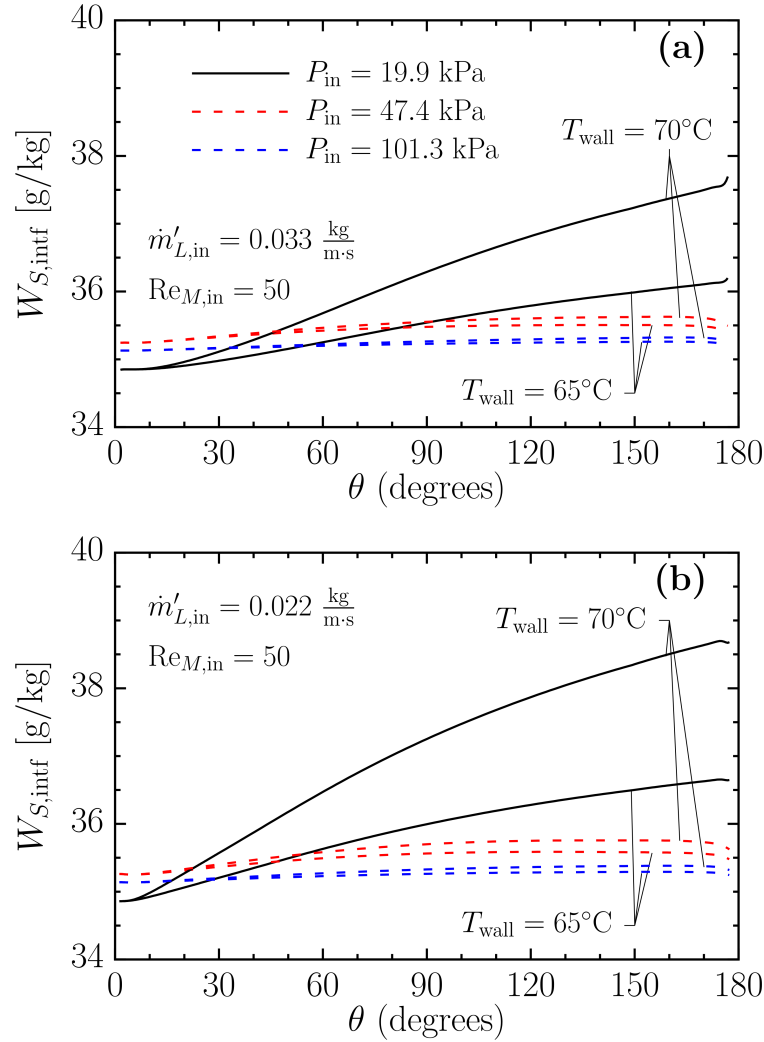


Figure 8.12: Interface salt mass fraction variation around the tube for different amounts of P_{in} , $\dot{m}'_{L,in}$, and T_{wall} .

8.4.3 Effects of $Re_{M,in}$ Variation on the Heat and Mass Transfer

To investigate the effects of mixture Reynolds number variation on the heat and mass transfer of the system, two cases are selected: one with a saturated inlet temperature ($P_{in} = 19.9$ kPa) and one with a sub-cooled inlet temperature ($P_{in} = 101.3$ kPa). The impacts of Reynolds number ($Re_{M,in}$) changes on the local heat transfer coefficient, total evaporated mass, and interface salt mass fraction are discussed below. Figure 8.13 shows the effects of $Re_{M,in}$ variation on the aforementioned parameters at $P_{in} = 19.9$ kPa. No significant changes are observed with increasing $Re_{M,in}$, indicating that varying the co-current gas flow velocity has minimal effect on heat and mass transfer at $P_{in} = 19.9$ kPa. Figure 8.14 shows the impacts of $Re_{M,in}$ variation on the same parameters at $P_{in} = 101.3$ kPa. The local heat transfer coefficient is not noticeably affected by $Re_{M,in}$. As depicted in Figure 8.14 (b), the total evaporated mass increases with $Re_{M,in}$. The total evaporated mass increases about 7% and 28% at the bottom of the tube when $Re_{M,in}$ increases from 25 to 50 and 100, respectively. Compared to the case with $P_{in} = 19.9$ kPa, this increase in the evaporation rate could be related to the concentration gradient at the interface being more affected by the bulk flow when air is present in the system. The interface salt mass fraction also slightly increases with a higher co-current mixture Reynolds number due to a higher evaporation rate, which raises the salt concentration at the interface.

8.4.4 Effects of Salinity Variation on the flow characteristics and Heat and Mass Transfer

To study the effects of inlet salinity on the flow, heat, and thermal characteristics of the system, a pure water falling film case is compared with two cases of salt water falling film with salinity of 35 g/kg and 70 g/kg at $P_{in} = 19.9$ kPa. Density and viscosity increase with salinity, while thermal conductivity, specific heat, and latent heat show a decreasing trend as salinity increases. Figure 8.15 depicts the variation in film thickness around the tube. The film thickness slightly

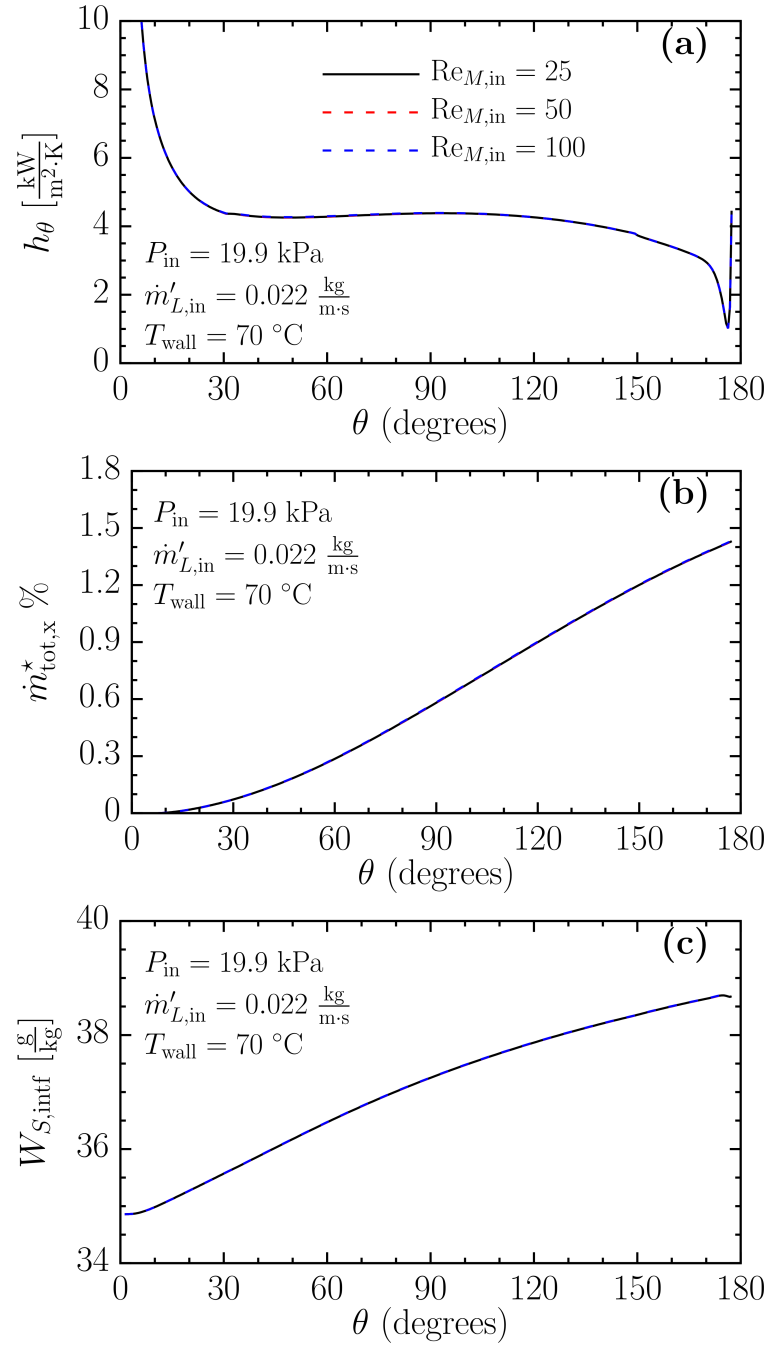


Figure 8.13: (a) Local heat transfer coefficient, (b) total evaporated mass, and (c) interface salt mass fraction variation around the tube for different amounts of $Re_{M,in}$ at $P_{in} = 19.9 \text{ kPa}$.

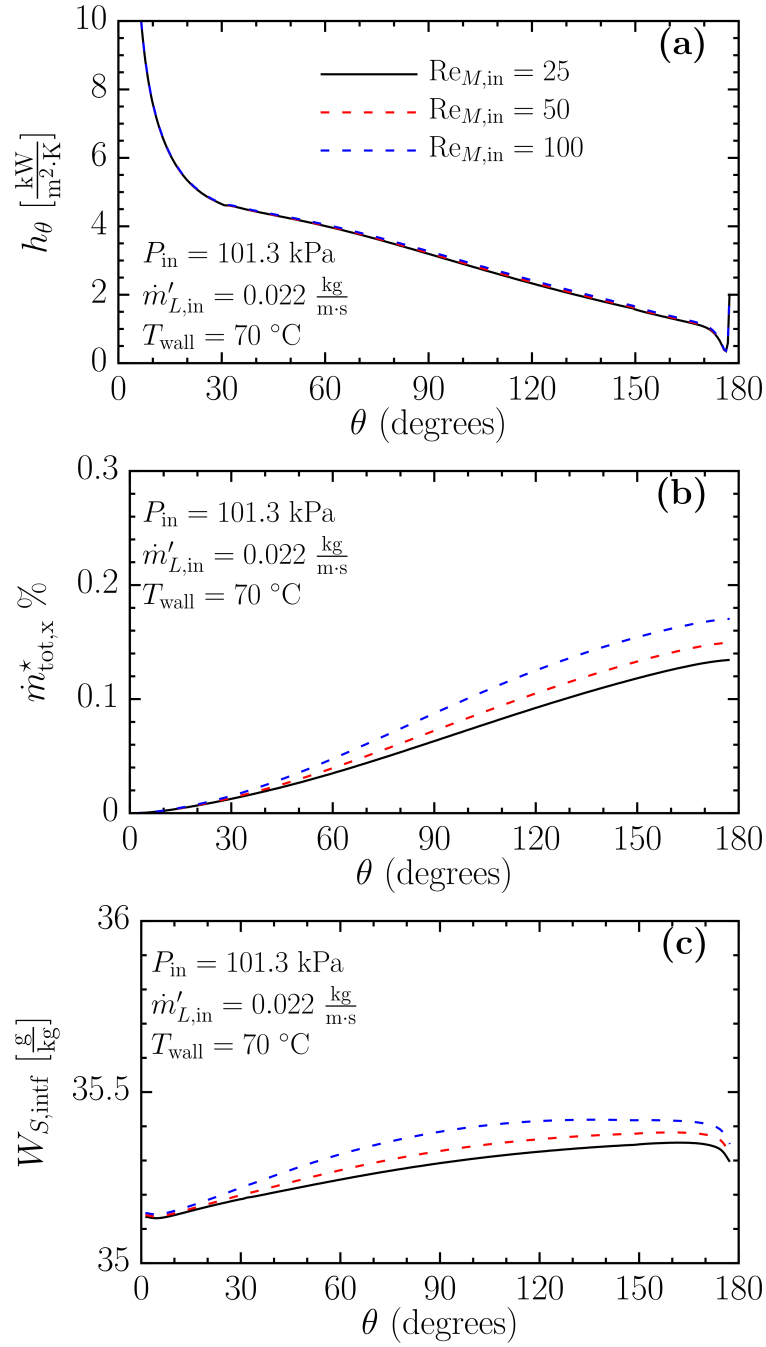


Figure 8.14: (a) Local heat transfer coefficient, (b) total evaporated mass, and (c) interface salt mass fraction variation around the tube for different amounts of $Re_{M,in}$ at $P_{in} = 101.3$ kPa.

increases with higher inlet salt mass fractions due to the increased liquid viscosity, which reduces the velocity and thickens the liquid film. This trend is consistent with the results found in the literature [66]. Figure 8.16 (a) shows the local heat transfer coefficient changes around the tube for different inlet salt mass fractions. Increasing the inlet salinity results in a decrease in h_θ around the tube. The same trend was observed in previous numerical and experimental studies [73, 94]. The increase in film thickness and decrease in thermal conductivity affect the liquid thermal conduction resistance, which limits heat transfer in the falling film. As shown in Figure 8.16 (b), the total evaporated mass decreases with increasing inlet salinity. Specifically, the total evaporated mass at the bottom of the tube decreases by about 6.5% and 9.7% when the inlet salt mass fraction increases to 35 g/kg and 70 g/kg, respectively. The evaporation of the liquid film also results in an increase in the interface salt mass fraction around the tube, as shown in Figure 8.16 (c). This increase is more pronounced for $W_{s,\text{in}} = 35$ g/kg.

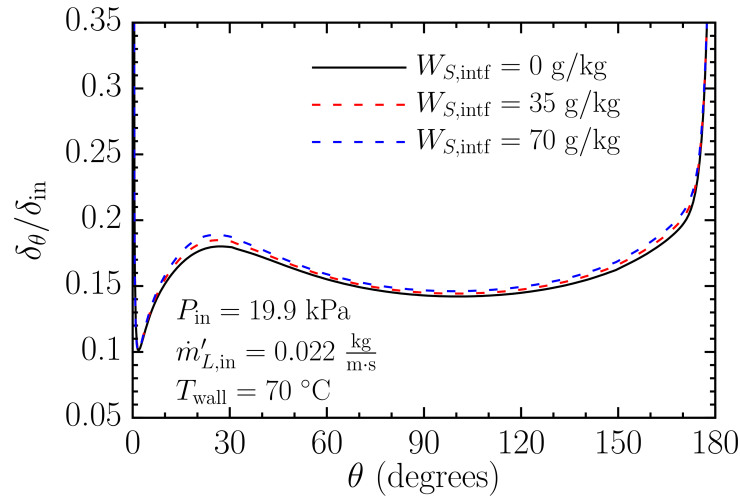
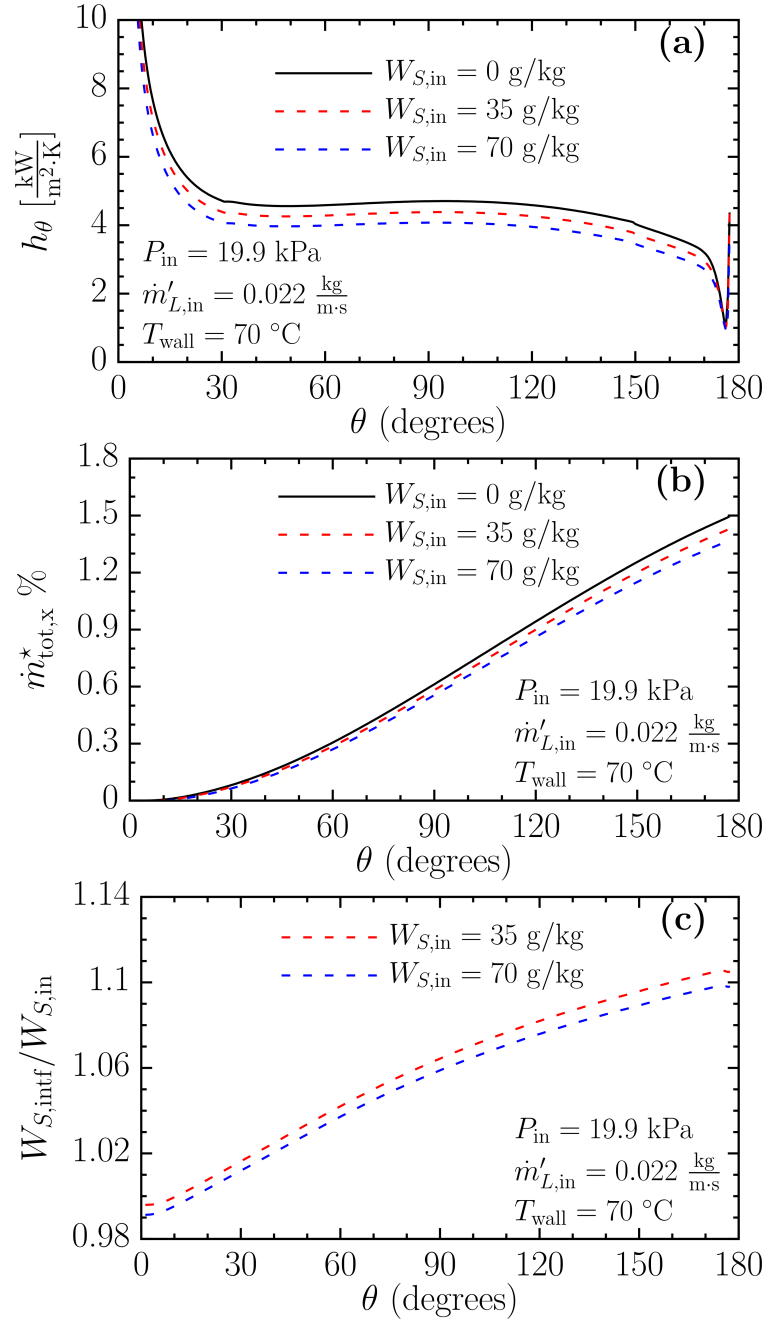


Figure 8.15: Film thickness variation around the tube for different amounts of W_S .


 Figure 8.16: Local heat transfer coefficient variation around the tube for different amounts of W_S .

Chapter 9

Concluding Remarks

9.1 Summary and Conclusions

In recent years, the desalination process has been recognized as a climate-independent source of producing potable water that has a great importance due to the lack of drinking water in many countries around the globe. One of the methods extensively used for removing salt from the sea-water is thermal distillation, which is known as a reliable technology for producing high-quality water by relying on the evaporation process. Among different evaporation methods, liquid falling film has been widely developed in the thermal desalination industry. In this method, the liquid falling film flows over a tube surface or inside a channel. During the evaporation process, the water vapour is separated from the saline water, which is collected later and turned into fresh liquid water; the remaining liquid leaves the system as a brine stream. In a desalination system, there are binary mixtures in the liquid and gas phases comprising salt-water and air-vapour, respectively. The presence of salt in the liquid mixture can affect the efficiency and performance of the evaporation process. Moreover, for the case of horizontal tube geometry, which is a popular set-up in the desalination industry, the creation of the recirculation zone in downstream of the tube can affect the flow and thermal characteristics of the system. Considerable experimental research has been conducted on the study of falling film desalination systems to investigate the heat and mass transfer over the horizontal tube geometry; however, the number of numerical studies is limited. Many of the numerical models found in the literature rely on the additional correlations for interface heat, mass, and momentum transfer. These correlations have a limited validity range, so their use is not always appropriate. Even most advanced numerical methods mostly utilized boundary layer approximation (parabolic approach) in their simulation, which is not capable of modelling the recirculation zones created at the flow downstream of the tube surface.

The key points that have not been sufficiently addressed in previous numerical studies of the evaporation process inside vertical channels and over horizontal tubes are:

- Utilizing a mass transfer model that is not based on empirical coefficients
- Sharp tracking of interface
- Consideration of fundamental force balances at the interface instead of using correlations
- Addressing the occurrence of supersaturation phenomenon in the mixture phase during the evaporation process
- Including the effect of variations of the thermophysical properties under the influence of temperature, pressure and salt and gas mass fraction changes

The main objective of the present work was to develop effective numerical models that properly addressed the limitations of the previous numerical methods and enhance understanding of the coupled momentum, heat, and mass transfer during the evaporation process through a comprehensive simulation of the two-phase flow phenomena inside vertical channels or on horizontal tubes. The two-phase fully-coupled parabolic and elliptic numerical models were utilized for the simulation of evaporation process inside vertical parallel plate channels. The elliptic approach was then applied for the simulation of desalination process inside vertical parallel plate channels and on horizontal tubes. Both models were able to capture the key features of flow as well as heat and mass transfer in the system. The parabolic model is more time-effective than the elliptic approach; however, the model is not capable of capturing reverse flow and recirculation zones.

The present study comprises four steps, and in each step the results have been validated against previous experimental and numerical data found in the literature. In the first step, a complete parabolic laminar two-phase flow model was developed to simulate the evaporation from a liquid falling film into a co-current gas mixture based on the conservation of momentum, mass, and energy. This model is believed to be the first evaporation application of a fully-coupled technique in

which all the field variables, the film thickness, and the pressure gradient are solved simultaneously. This technique provides robust solution behaviour and fast convergence. Fundamental balances of energy, mass, and shear force at the interface assured the proper interaction between the liquid and mixture phases. The governing equations were discretized using a finite volume method. A robust fully coupled solution approach was used to solve the resulting algebraic equations in a marching scheme along the channel. The liquid-gas interface location was coincident with the mesh at every axial station in the solution. The solution fields included the axial velocity, transverse mass flux, and temperature for both phases plus the air mass fraction, the film thickness, and the axial pressure gradient. The model validity was demonstrated by comparisons with previous numerical and experimental works. Trends in the evaporation rate and local field profiles have been discussed in more detail than previous studies. In the present study, the field variables affecting the evaporation rate near the channel inlet were discussed and the effect of buoyancy forces on the velocity profile was examined. New findings discussing the effects of inlet pressure change on the flow, heat, and mass characteristics during the evaporation process were also presented. A system effectiveness was defined, and the impact of changes to the inlet liquid Reynolds number and pressure on the effectiveness were examined. The present model predictions indicate that:

1. The high level of evaporation rate near the inlet is mainly due to the concentration difference between the liquid and mixture. The heat and mass fluxes then experience a sharp decrease up to $x/H = 1$ due to the decrease of mass fraction gradient at the interface.
2. An inlet pressure increase intensifies the effects thermal opposing buoyancy forces, leading to a flow deceleration near the interface.
3. The pressure increase also decreases the interfacial heat and mass flux, which reduces the evaporation rate.
4. The system effectiveness decreases by increasing the inlet liquid Reynolds number and inlet pressure.

In the second step, the numerical model utilized an elliptic approach to study the laminar two-phase flow phenomenon of the evaporation of pure water falling film into a co-current gas mixture. A finite volume method was used to obtain a fully coupled implicit solution of a complete set of elliptic two-dimensional governing equations. The equations for mass, momentum, gas mass fraction, and energy were solved on a co-located structured non-orthogonal grid for both the liquid and gas phases. The pressure field was implicitly computed for the entire domain. A pressure-weighted interpolation method (PWIM) was applied to estimate the face velocities and to provide implicit pressure-velocity coupling via the continuity equation. The solution field variables, including the axial velocity, transverse velocity, pressure, and temperature for both phases, plus the air mass fraction for the gas phase were solved simultaneously in the entire domain. Once all solution variables are computed on a fixed grid, the interface location is sharply determined by imposing mass balance at the end of each time step for all liquid columns within the domain. This precise interface resolution enables more accurate determinations of the interface location, interfacial shear stress, and velocity profiles compared to methods such as VOF, where the interface is estimated in control volumes by varying the volume fractions from zero to one. The iterative procedure continues until a steady state solution convergence is obtained. The excess moisture condensation (EMC) model was also introduced as a novel method to address supersaturation in the system. Detailed comparisons with previous numerical works demonstrated the validity of the present model. A water-air mixture was used to examine the effects of buoyancy forces on the flow and the thermal characteristics of the evaporation process inside a partially heated vertical parallel plate channel. The impact of changes to the $Re_{L,in}$ and $Re_{M,in}$ on the flow features, evaporation rate, and the effectiveness of the system were studied. The present model predictions indicate that:

1. A supersaturation up to 15% does not affect the field variables significantly.
2. For low liquid and mixture Re numbers, the opposing buoyancy forces can dominate the aiding forces, and a flow reversal occurs close to the interface at the heated section.
3. At the insulated section, the low evaporation rate and the diffusion of air towards the interface

weaken the opposing forces leading to the creation of recirculation zones in the system.

4. The creation of a recirculation zone affects the interfacial heat and mass flux at the heated section due to the strong flow reversal that occurs close to the interface.
5. The system effectiveness increases by reducing the inlet liquid Reynolds number and increasing the mixture Reynolds number.

In the third step, the elliptic model was developed to study the flow and thermal characteristics of the evaporation process of seawater inside a vertical parallel plate channel. To the best knowledge of the author, the implementation of an elliptic approach to a two-phase falling film desalination process inside a vertical parallel plate channel had not been previously addressed. Therefore, elliptic model was used investigate the effects of mixed convection and salt concentration on the flow and thermal characteristics of the evaporation process of liquid saline water film within a vertical parallel plate channel. To achieve this aim, a salt mass fraction equation was solved along with other above-mentioned equations. The partial enthalpy related transport advection terms were added to the liquid energy conservation equation. This was a new feature that had not been used in the previous desalination studies. Moreover, liquid phase equations and interface conditions were updated to model a binary liquid mixture. The validity of the present model was assessed through comparisons with a previous experimental study for pure water evaporation. The influences of changes to the $Re_{L,in}$, S_{in} , q''_{wall} , and ϕ_{in} on flow characteristics, evaporation rate, and system effectiveness were examined. The predictions obtained from the model suggest that:

1. The evaporation rate and effectiveness increase with increased wall heat flux and reduced inlet liquid Reynolds number.
2. An increase in the inlet salinity leads to a reduction in the interfacial evaporation rate.
3. The effects of q''_{wall} and $Re_{L,in}$ changes on the flow, heat transfer, and mass transfer, more pronounced than the effects of changes in S_{in} .

4. The evaporation rate and interfacial transport variables are not significantly affected by changing the inlet air relative humidity.

In the last step, the research was extended to model the evaporation of fresh water and salt water falling film over a horizontal tube. The elliptic approach which is capable of capturing the re-circulation zones was used for the simulations. To the best knowledge of the author, the elliptic model developed in the present study offers a more comprehensive and detailed approach compared to any previous numerical studies on falling film evaporation. The results were compared to the previous experimental and numerical studies for both pure and salt water falling films. The results of a parametric study indicates that:

1. The presence of non-condensable gas in the mixture phase negatively affected the evaporation rate.
2. The decrease of the liquid mass flow rate thins the liquid film and improves the heat transfer and evaporation rate of the system.
3. The increase of the wall temperature increases the heat and mass transfer in the system.
4. The variation of the mixture Reynolds number has the minimum impact on the flow characteristics and evaporation rate.
5. Increase of salinity in the liquid affects the heat transfer and evaporation rate through the changes of the liquid thermophysical properties.

9.2 Recommendation for Future Works

To improve the capability and performance of the elliptic numerical model and to examine its potential the following future work is recommended:

- **Study the desalination process on tube bundles:** In a falling film evaporator with a large-scale tube bundle, the heat transfer coefficient of each individual tube varies depending on its position within the bundle. The study of various tube configurations and the flow pattern transitions between the tubes could help to better understand the process for practical applications in desalination industry.
- **Add turbulence models to the liquid and gas phase equations:** Implementing a turbulence model for the liquid and gas regions would enable the simulation of flows at higher Reynolds numbers and facilitate the exploration of falling film characteristics over a wider range of mass flow rates.
- **Apply effective iterative solvers to improve the model efficiency:** The system of equations in the elliptic two-phase model is ill-conditioned due to the strong coupling of solution variables at the interface. Not all iterative solvers can handle such a system effectively. While the direct solvers used in this study were able to solve this type of equation, they were not computationally efficient. To take advantage of the benefits of both solver types, one could use iterative solvers for the gas and liquid regions, followed by a direct solver for the interface equations.
- **Couple the interface and mesh movement into the system of equations:** Determining the interface location could be implicitly integrated with the solution for the field variables. Utilizing a geometric conservation law as the governing equation for both the interface and mesh movement, and coupling it with all other equations, could facilitate faster convergence.
- **Include the surface tension in the interface force balance:** Developing a robust, coupled calculation of the surface tension could improve the prediction of liquid falling film specifically in the upper and lower stagnation points locations.

References

- [1] W. Yan, T. Lin and Y. Tsay, Evaporative cooling of liquid film through interfacial heat and mass transfer in a vertical channel—i. experimental study, *International Journal of Heat and Mass Transfer* **34**(4-5) (1991), 1105–1111.
- [2] X. Chen, S. Shen, Y. Wang, J. Chen and J. Zhang, Measurement on falling film thickness distribution around horizontal tube with laser-induced fluorescence technology, *International Journal of Heat and Mass Transfer* **89** (2015), 707–713.
- [3] J. Wang, X. Chen, T. Lu, X. Chen, S. Shen and B. Liu, Three-dimensional film thickness distribution of horizontal tube falling film with column flow, *Applied Thermal Engineering* **154** (2019), 140–149.
- [4] X. Hu and A. Jacobi, The intertube falling film: Part 2—mode effects on sensible heat transfer to a falling liquid film, *ASME Journal of Heat and Mass Transfer* **118** (1996).
- [5] S. Shen, X. Chen, X. Mu and C. Jiang, Experimental studies on heat transfer coefficients of horizontal tube falling film evaporation with seawater, *Journal of Heat Transfer* **139**(1) (2017).
- [6] C. Chang, T. Lin and W. Yan, Natural convection flows in a vertical, open tube resulting from combined buoyancy effects of thermal and mass diffusion, *International Journal of Heat and Mass Transfer* **29**(10) (1986), 1543–1552.
- [7] T. Lin, C. Chang and W. M. Yan, Analysis of combined buoyancy effects of thermal and mass diffusion on laminar forced convection heat transfer in a vertical tube, *Journal of Heat Transfer* **110**(2) (1988), 337–344.
- [8] W. Yan, Y. Tsay and T. Lin, Simultaneous heat and mass transfer in laminar mixed convection flows between vertical parallel plates with asymmetric heating, *International Journal of Heat and Fluid Flow* **10**(3) (1989), 262–269.

References

- [9] W.-M. Yan, Effects of film evaporation on laminar mixed convection heat and mass transfer in a vertical channel, *International Journal of Heat and Mass Transfer* **35**(12) (1992), 3419–3429.
- [10] W.-M. Yan, Binary diffusion and heat transfer in mixed convection pipe flows with film evaporation, *International Journal of Heat and Mass Transfer* **36**(8) (1993), 2115–2123.
- [11] W.-M. Yan and C.-Y. Soong, Numerical study of liquid film cooling along an inclined plate, *Wärme Und Stoffübertragung* **28**(4) (1993), 233–241.
- [12] W.-M. Yan and S. Chyi-Yeou, Numerical study of liquid film cooling in a turbulent gas stream, *International Journal of Heat and Mass Transfer* **36**(16) (1993), 3877–3885.
- [13] W.-M. Yan, Convective heat and mass transfer from a falling film to a laminar gas stream, *Wärme Und Stoffübertragung* **29**(2) (1993), 79–87.
- [14] W.-M. Yan and C.-Y. Soong, Convective heat and mass transfer along an inclined heated plate with film evaporation, *International Journal of Heat and Mass Transfer* **38**(7) (1995), 1261–1269.
- [15] Y. Tsay, T. Lin and W. Yan, Cooling of a falling liquid film through interfacial heat and mass transfer, *International Journal of Multiphase Flow* **16**(5) (1990), 853–865.
- [16] Y. Tsay and T. Lin, Evaporation of a heated falling liquid film into a laminar gas stream, *Experimental Thermal and Fluid Science* **11**(1) (1995), 61–71.
- [17] S. He, P. An, J. Li and J. Jackson, Combined heat and mass transfer in a uniformly heated vertical tube with water film cooling, *International Journal of Heat and Fluid Flow* **19**(5) (1998), 401–417.
- [18] M. Feddaoui, E. Belahmidi, A. Mir and A. Bendou, Numerical study of the evaporative cooling of liquid film in laminar mixed convection tube flows, *International Journal of Thermal Sciences* **40**(11) (2001), 1011–1020.

- [19] M. Feddaoui, A. Mir and E. Belahmidi, Cocurrent turbulent mixed convection heat and mass transfer in falling film of water inside a vertical heated tube, *International Journal of Heat and Mass Transfer* **46**(18) (2003), 3497–3509.
- [20] M. Feddaoui, A. Mir and E. Belahmidi, Numerical simulation of mixed convection heat and mass transfer with liquid film cooling along an insulated vertical channel, *Heat and Mass Transfer* **39**(5) (2003), 445–453.
- [21] M. Feddaoui, H. Meftah and A. Mir, The numerical computation of the evaporative cooling of falling water film in turbulent mixed convection inside a vertical tube, *International Communications in Heat and Mass Transfer* **33**(7) (2006), 917–927.
- [22] M. Feddaoui and A. Mir, Turbulent mixed convection heat and mass exchanges in evaporating liquid film along a vertical tube, *International Journal of Heat Exchangers* **7**(1) (2007), 15–30.
- [23] H. Raach and J. Mitrovic, Seawater falling film evaporation on vertical plates with turbulence wires, *Desalination* **183**(1-3) (2005), 307–316.
- [24] H. Raach and J. Mitrovic, Simulation of heat and mass transfer in a multi-effect distillation plant for seawater desalination, *Desalination* **204**(1-3) (2007), 416–422.
- [25] A. Nasr, C. D. Hfaiedh and S. B. Nasrallah, Numerical study of evaporation by mixed convection of a binary liquid film, *Energy* **36**(5) (2011), 2316–2327.
- [26] A. Nait Alla, M. Feddaoui and H. Meftah, Numerical study of the evaporation by mixed convection of ethanol in partially heated plate along a vertical channel, *International Journal of Heat and Mass Transfer* **89** (2015), 206–215.
- [27] C. Ren and Y. Wan, A new approach to the analysis of heat and mass transfer characteristics for laminar air flow inside vertical plate channels with falling water film evaporation, *International Journal of Heat and Mass Transfer* **103** (2016), 1017–1028.

- [28] M. Najim, M. Feddaoui, A. Charef and H. Meftah, Computational study of saline water film evaporation in a vertical tube, *Desalination* **408** (2017), 81–91.
- [29] M. Najim, M. Feddaoui, A. Nait Alla, A. Charef and A. E. Kabeel, New cooling approach using successive evaporation and condensation of a liquid film inside a vertical mini-channel, *International Journal of Heat and Mass Transfer* **122** (2018), 895–912.
- [30] A. Nait Alla, H. Meftah et al., Comparison of two configurations to improve heat and mass transfer in evaporating two-component liquid film flow, *International Journal of Thermal Sciences* **126** (2018), 194–204.
- [31] A. Nait Alla, M. Feddaoui and M. Najim, Falling film evaporation of ternary mixture under three different modes of heating, *Heat Transfer* **50**(8) (2021), 7839–7854.
- [32] Y. Tohidi and S. Ormiston, Numerical analysis of evaporation from a falling film in a vertical parallel plate channel, *International Journal of Heat and Mass Transfer* **196** (2022).
- [33] Y. Tohidi and S. Ormiston, Falling film evaporation in a partially heated parallel plate channel: Elliptic numerical analysis with an excess moisture condensation model, *International Journal of Heat and Mass Transfer* **210** (2023), 124174.
- [34] A. N. Alla, L. Bammou, S. Alami, M. Najim, A. Charef, S. Bouchta, M. Errai and M. Feddaoui, Effect of nanoparticles on the evaporation of a salt water film, *International Journal of Low-Carbon Technologies* **18** (2023), 600–608.
- [35] Y. Tohidi and S. Ormiston, A two-phase sharp-interface numerical model of falling film thermal desalination in a vertical channel, *Heat and Mass Transfer* (2024, Accepted).
- [36] J. Mitrovic, Influence of tube spacing and flow rate on heat transfer from a horizontal tube to a falling liquid film, in *International Heat Transfer Conference Digital Library*, Begel House Inc. (1986).

- [37] Q. Qiu, C. Meng, S. Quan and W. Wang, 3-d simulation of flow behaviour and film distribution outside a horizontal tube, *International Journal of Heat and Mass Transfer* **107** (2017), 1028–1034.
- [38] A. Karmakar and S. Acharya, Numerical simulation of falling film flow hydrodynamics over round horizontal tubes, *International Journal of Heat and Mass Transfer* **173** (2021), 121175.
- [39] F. Sun, S. Xu and Y. Gao, Numerical simulation of liquid falling film on horizontal circular tubes, *Frontiers of chemical science and engineering* **6** (2012), 322–328.
- [40] Q. Qiu, X. Zhu, L. Mu and S. Shen, An investigation on the falling film thickness of sheet flow over a completely wetted horizontal round tube surface, *Desalination and Water Treatment* **57**(35) (2016), 16277–16287.
- [41] Q. Qiu, X. Zhu, L. Mu and S. Shen, Numerical study of falling film thickness over fully wetted horizontal round tube, *International Journal of Heat and Mass Transfer* **84** (2015), 893–897.
- [42] I. Hassan, A. Sadikin and N. M. Isa, The computational modeling of falling film thickness flowing over evaporator tubes, *Journal of Advanced Research in Fluid Mechanics and Thermal Sciences* **14**(1) (2015), 24–37.
- [43] M. Li, Y. Lu, S. Zhang and Y. Xiao, A numerical study of effects of counter-current gas flow rate on local hydrodynamic characteristics of falling films over horizontal tubes, *Desalination* **383** (2016), 68–80.
- [44] H. Han, C. Sun, Y. Wang and Y. Li, Numerical simulation of horizontal tube falling film flow under tilt and sloshing conditions, *Energy Procedia* **142** (2017), 3888–3894.

- [45] S. Lin, Z. Zhang, X. Liu, K. Zhuang and X. Li, Numerical study of falling film flow on a horizontal rotating tube, *International Journal of Heat and Mass Transfer* **117** (2018), 465–473.
- [46] Q. Qiu, X. Zhang, S. Quan, X. Zhu and S. Shen, 3d numerical study of the liquid film distribution on the surface of a horizontal-tube falling-film evaporator, *International Journal of Heat and Mass Transfer* **124** (2018), 943–952.
- [47] X. Zhang, C. Meng, Q. Qiu, S. Quan and S. Shen, A numerical investigation of liquid film flow and film thickness distribution outside a horizontal tube, *International Journal of Low-Carbon Technologies* **13**(4) (2018), 424–431.
- [48] C.-Y. Zhao, W.-T. Ji, P.-H. Jin, Y.-J. Zhong and W.-Q. Tao, Hydrodynamic behaviors of the falling film flow on a horizontal tube and construction of new film thickness correlation, *International Journal of Heat and Mass Transfer* **119** (2018), 564–576.
- [49] H. Han, S. Wang, T. He, Y. Li and C. Sun, Numerical study of the falling film thickness around the tube bundle with different spacings between spray holes and tubes under tilt and sloshing conditions, *International Journal of Heat and Mass Transfer* **138** (2019), 184–193.
- [50] A. Kumar Poddar and N. Singh, Numerical study of liquid film formation around tubes of horizontal falling film evaporator, *Journal of Applied Fluid Mechanics* **14**(4) (2021), 1045–1052.
- [51] F. Tahir, A. Mabrouk and M. Koç, Influence of co-current vapor flow on falling film over horizontal tube, *International Journal of Thermal Sciences* **159** (2021), 106614.
- [52] M. Zhou, P. Tao, X. Di and J. Zhou, Numerical study on the effect of co-current gas flow on the falling film flow characteristics outside the horizontal tube, *Nuclear Engineering and Design* **413** (2023), 112510.

- [53] G. Kocamustafaogullari and I. Chen, Falling film heat transfer analysis on a bank of horizontal tube evaporator, *AIChE Journal* **34**(9) (1988), 1539–1549.
- [54] K. Bourouni, M. Chaibi and L. Tadrist, Analytical analysis of heat transfer in liquid film dripping around a horizontal tube, *Desalination* **141**(1) (2001), 7–13.
- [55] W. K. Hu, L. Yang and L. H. Guo, Numerical simulation of the liquid flowing and heat-transfer outside the tube of the horizontal-tube falling film evaporator, *Advanced Materials Research* **614** (2013), 296–300.
- [56] L. Yang, C. Xue, B. Zhang, K. Zhang and S. Tao, Numerical analysis of thermodynamic behaviour of falling film outside a horizontal tube, *Desalination and Water Treatment* **51**(4-6) (2013), 872–876.
- [57] M.-C. Chyu and A. Bergles, An analytical and experimental study of falling-film evaporation on a horizontal tube, *Journal of Heat Transfer* **109**(4) (1987), 983–990.
- [58] L. Yang, Y. Liu, Y. Yang and S. Shen, Microscopic mechanisms of heat transfer in horizontal-tube falling film evaporation, *Desalination* **394** (2016), 64–71.
- [59] C.-h. Qi, H.-j. Feng, H.-q. Lv and C. Miao, Numerical and experimental research on the heat transfer of seawater desalination with liquid film outside elliptical tube, *International Journal of Heat and Mass Transfer* **93** (2016), 207–216.
- [60] A. Karmakar and S. Acharya, Heat transfer characteristics of falling film over horizontal tubes-a numerical study, in *55th AIAA Aerospace Sciences Meeting*, p. 0901 (2017).
- [61] F. Wunder, S. Enders and R. Semiat, Numerical simulation of heat transfer in a horizontal falling film evaporator of multiple-effect distillation, *Desalination* **401** (2017), 206–229.
- [62] C.-Y. Zhao, W.-T. Ji, Y.-L. He, Y.-J. Zhong and W.-Q. Tao, A comprehensive numerical study on the subcooled falling film heat transfer on a horizontal smooth tube, *International Journal of Heat and Mass Transfer* **119** (2018), 259–270.

- [63] M. Ning, J. Hao, T. He, Y. Xu, M. Song and J. Tang, Unsteady heat transfer properties of spray falling over a horizontal tube in an oily sewage source heat pump, *Applied Thermal Engineering* **179** (2020), 115675.
- [64] M. Ning, H. Jingyu, X. Yingjie, S. Mengjie and T. Jianfeng, A numerical study on non-uniform characteristics of spray falling heat transfer over horizontal tubes in an oily sewage source heat pump, *International Journal of Heat and Mass Transfer* **154** (2020), 119679.
- [65] F. Tahir, A. Mabrouk and M. Koç, Heat transfer coefficient estimation of falling film for horizontal tube multi-effect desalination evaporator using cfd, *International Journal of Thermofluids* **11** (2021), 100101.
- [66] Z. Wan, Y. Li and S. Wang, A comprehensive simulation and optimization on heat transfer characteristics of subcooled seawater falling film around elliptical tubes, *Applied Thermal Engineering* **189** (2021), 116675.
- [67] H. Zhang and Y. Zhou, Effects of tube shape on the distribution of film thickness and heat transfer performance in falling film evaporation, *Heat and Mass Transfer* **58**(9) (2022), 1533–1543.
- [68] K. Bourouni, R. Martin, L. Tadrist and H. Tadrist, Modelling of heat and mass transfer in a horizontal-tube falling-film evaporator for water desalination, *Desalination* **116**(2-3) (1998), 165–183.
- [69] J. Hao, Y. Xu, T. He, N. Mao, M. Song and J. Tang, Numerical study on heat transfer of oily wastewater spray falling film over a horizontal tube in a sewage source heat pump, *International Journal of Heat and Mass Transfer* **142** (2019), 118423.
- [70] A. Al-Ansari and I. Owen, Thermal and hydrodynamic analysis of the condensation and evaporation processes in horizontal tube desalination plant, *International Journal of Heat and Mass Transfer* **42**(9) (1999), 1633–1644.

- [71] R. Kouhikamali, S. N. R. Abadi and M. Hassani, Numerical investigation of falling film evaporation of multi-effect desalination plant, *Applied thermal engineering* **70**(1) (2014), 477–485.
- [72] S. Bigham, R. KouhiKamali and S. Noori Rahim Abadi, Two-phase flow numerical simulation and experimental verification of falling film evaporation on a horizontal tube bundle, *Desalination and Water Treatment* **55**(8) (2015), 2009–2022.
- [73] R. Abraham and A. Mani, Heat transfer characteristics in horizontal tube bundles for falling film evaporation in multi-effect desalination system, *Desalination* **375** (2015), 129–137.
- [74] S. Lin, X. Liu and X. Li, The spatial distribution of liquid film thickness outside the horizontal falling film tube, *International Journal of Heat and Mass Transfer* **143** (2019), 118577.
- [75] D. Balaji, R. Velraj and R. Murthy, Numerical investigation on the effect of tube geometry and feeder height on the heat transfer performance of horizontal tube falling film evaporation, *Journal of Heat Transfer* **141**(11) (2019), 111502.
- [76] D. Balaji, R. Velraj and M. Ramana Murthy, Numerical studies on the thermal regimes of the horizontal tube falling film evaporation under varying feeder height, *International Journal of Green Energy* **17**(14) (2020), 895–911.
- [77] F. Tahir, A. Mabrouk and M. Koç, Impact of surface tension and viscosity on falling film thickness in multi-effect desalination (med) horizontal tube evaporator, *International Journal of Thermal Sciences* **150** (2020), 106235.
- [78] L. Yang, L. Zhang, A. Li and J. Wu, Modeling thermal and geometrical effects on non-condensable gas desorption in horizontal-tube bundles of falling film evaporation, *Desalination* **478** (2020), 114302.
- [79] F. Tahir, A. Mabrouk and M. Koc, Review on cfd analysis of horizontal falling film evaporators in multi effect desalination plants, *Desalin. Water Treat* **166** (2019), 296–320.

- [80] Q. Wang, M. Li, W. Xu, L. Yao, X. Liu, D. Su and P. Wang, Review on liquid film flow and heat transfer characteristics outside horizontal tube falling film evaporator: Cfd numerical simulation, *International Journal of Heat and Mass Transfer* **163** (2020), 120440.
- [81] Z. Dai, Y. Zhang, S. Wang, K. Nawaz and A. Jacobi, Falling-film heat exchangers used in desalination systems: A review, *International Journal of Heat and Mass Transfer* **185** (2022), 122407.
- [82] C.-Y. Zhao, C.-M. Zheng, X.-S. Wang, D. Qi, J.-M. Jiang, W.-T. Ji, P.-H. Jin and W.-Q. Tao, Correlations of falling film hydrodynamics and heat transfer on horizontal tubes: A review, *Renewable and Sustainable Energy Reviews* **197** (2024), 114384.
- [83] M. Fiorentino and G. Starace, Numerical investigations on two-phase flow modes in evaporative condensers, *Applied Thermal Engineering* **94** (2016), 777–785.
- [84] X. Xie, H. Liu, C. He, B. Zhang, Q. Chen and M. Pan, Deciphering the heat and mass transfer behaviors of staggered tube bundles in a closed wet cooling tower using a 3-d vof model, *Applied Thermal Engineering* **161** (2019), 114202.
- [85] L. S. Fletcher, V. Sernas and W. H. Parken, Evaporation heat transfer coefficients for thin sea water films on horizontal tubes, *Industrial & Engineering Chemistry Process Design and Development* **14**(4) (1975), 411–416.
- [86] W. Parken, L. Fletcher, V. Sernas and J. Han, Heat transfer through falling film evaporation and boiling on horizontal tubes, *ASME Journal of Heat and Mass Transfer* **112** (1990).
- [87] X. Hu and A. Jacobi, The intertube falling film: Part 1—flow characteristics, mode transitions, and hysteresis, *ASME Journal of Heat and Mass Transfer* **118** (1996).
- [88] Y. Fujita and M. Tsutsui, Experimental investigation of falling film evaporation on horizontal tubes, *Heat Transfer-Japanese Research: Co-sponsored by the Society of Chemical Engineers of Japan and the Heat Transfer Division of ASME* **27**(8) (1998), 609–618.

- [89] D. Gstoehl, J. Roques, P. Crisinel and J. Thome, Measurement of falling film thickness around a horizontal tube using a laser measurement technique, *Heat Transfer Engineering* **25**(8) (2004), 28–34.
- [90] L. Yang and S. Shen, Experimental study of falling film evaporation heat transfer outside horizontal tubes, *Desalination* **220**(1-3) (2008), 654–660.
- [91] H. Hou, Q. Bi, H. Ma and G. Wu, Distribution characteristics of falling film thickness around a horizontal tube, *Desalination* **285** (2012), 393–398.
- [92] X. Mu, S. Shen, Y. Yang and X. Liu, Experimental study of falling film evaporation heat transfer coefficient on horizontal tube, *Desalination and Water Treatment* **50**(1-3) (2012), 310–316.
- [93] B. Narvaez-Romo and J. R. Simoes-Moreira, Falling liquid film evaporation in subcooled and saturated water over horizontal heated tubes, *Heat Transfer Engineering* **38**(3) (2017), 361–376.
- [94] C. Li, L. Zhang, X. Mu, X. Chen and S. Shen, A correlation of heat transfer for falling film evaporation on the horizontal tube with multiple-precision expansion method, *International Journal of Heat and Mass Transfer* **221** (2024), 125022.
- [95] E. C. Siow, Numerical solution of a two-phase model for laminar film condensation of vapour-gas mixtures in channels, M.Sc. thesis, University of Manitoba, Department of Mechanical and Industrial Engineering (July 2001).
- [96] F. Hassaninejadfarahani, M. K. Guyot and S. J. Ormiston, Numerical analysis of mixed-convection laminar film condensation from high air mass fraction steam-air mixtures in vertical tubes, *International Journal of Heat and Mass Transfer* **78** (2014), 170–180.

References

- [97] Y. Q. Wang, L. Penner and S. Ormiston, Analysis of laminar forced convection of air for crossflow in banks of staggered tubes, *Numerical Heat Transfer: Part A: Applications* **38**(8) (2000), 819–845.
- [98] S. V. Patankar, *Numerical heat transfer and fluid flow*, Hemisphere Publishing Corporation (1980).
- [99] A. Behie, D. Collins, J. Forsyth, P. A. and P. H. Sammon, Fully coupled multiblock wells in oil simulation, *Society of Petroleum Engineers Journal* **25**(04) (Aug. 1985), 535–542.
- [100] C. M. Rhie and W. L. Chow, Numerical study of the turbulent flow past an airfoil with trailing edge separation, *AIAA Journal* **21**(11) (1983), 1525–1532.
- [101] G. D. Raithby and G. E. Schneider, *Elliptic systems: Finite-difference method II*, *Handbook of Numerical Heat Transfer*, edited by W. J. Minkowycz, E. M. Sparrow, G. E. Schneider and R. H. Pletcher, John Wiley & Sons (1988).
- [102] J. Van Doormaal and C. Raithby, Enhancements of the simple method for predicting incompressible fluid flows, *Numerical Heat Transfer* **7** (1984), 147–163.
- [103] X. S. L and J. W. Demmel, Superlu-dist: A scalable distributed-memory sparse direct solver for unsymmetric linear systems, *ACM Trans. Math. Softw.* **29**(2) (June 2003), 110–140.
- [104] W. Yan and T. Lin, Evaporative cooling of liquid film through interfacial heat and mass transfer in a vertical channel—ii. numerical study, *International Journal of Heat and Mass Transfer* **34**(4-5) (1991), 1113–1124.
- [105] W. Yan and T. Lin, Combined heat and mass transfer in natural convection between vertical parallel plates with film evaporation, *International Journal of Heat and Mass Transfer* **33**(3) (1990), 529–541.

References

- [106] R. Abbasi Havestini and S. J. Ormiston, Detailed two-phase numerical analysis of falling film absorption over a horizontal tube, *International Journal of Heat and Mass Transfer* **198** (2022), 123378.
- [107] M. H. Sharqawy, J. H. Lienhard and S. M. Zubair, Thermophysical properties of seawater: a review of existing correlations and data, *Desalination and Water Treatment* **16**(1-3) (2010), 354–380.
- [108] J. K. Min and D. H. Choi, Analysis of the absorption process on a horizontal tube using Navier-Stokes equations with surface-tension effects, *International Journal of Heat and Mass Transfer* **42** (Dec. 1999), 4567–4578.
- [109] J. Mitrovic, Preventing formation of dry patches in seawater falling film evaporators, *Desalination and Water Treatment* **29**(1-3) (2011), 149–157.
- [110] H. Louahlia-Gualous and L. E. Omari, Local heat transfer for the evaporation of a laminar falling liquid film on a cylinder: experimental, numerical, and inverse heat conduction analysis, *Numerical Heat Transfer, Part A: Applications* **50**(7) (2006), 667–688.
- [111] E. A. Saleh and S. J. Ormiston, A sharp-interface elliptic numerical model of laminar two-phase gas-liquid downward flow in a vertical parallel plate channel, *The Canadian Journal of Chemical Engineering* **95**(3) (Mar. 2017), 568–577.
- [112] R. B. Stull, C. D. Ahrens et al., *Meteorology for Scientists and Engineers*, Brooks/Cole (2000).
- [113] V. P. Carey, *Liquid-vapor Phase-change Phenomena: an Introduction to the Thermophysics of Vaporization and Condensation Processes in Heat Transfer Equipment*, CRC Press (2020).
- [114] L. A. Bromley, D. Singh, P. Ray, S. Sridhar and S. M. Read, Thermodynamic properties of sea salt solutions, *AIChE Journal* **20**(2) (1974), 326–335.

Contributions

- **Yasaman Tohidi**, Scott J. Ormiston “Detailed Numerical Analysis of Falling Film Thermal Desalination in a Vertical Channel”, *Heat and Mass Transfer*, Published, Volume 61 (2025)
- **Yasaman Tohidi**, Scott J. Ormiston “Falling film evaporation in a partially heated parallel plate channel: Elliptic numerical analysis with an excess moisture condensation model”, *International Journal of Heat and Mass Transfer*, Published, Volume 210 (2023)
- **Yasaman Tohidi**, Scott J. Ormiston “Numerical analysis of evaporation from a falling film in a vertical parallel plate channel”, *International Journal of Heat and Mass Transfer*, Published, Volume 196 (2022)
- Shidvash Vakilipour, **Yasaman Tohidi**, Jafar Al-Zaili, and Rouzbeh Riazi “The Thermochemical Effects of CO₂ Dilution on the Combustion Characteristics of a Swirl Stabilized Diffusion Flame”, *Applied Mathematics and Mechanics*, Published, Volume 41 (2020)
- **Yasaman Tohidi** and Shidvash Vakilipour “A Numerical Study on the Effects of N₂ Dilution on the Flame Structure and Temperature Distribution of Swirl Diffusion Flames”, *International Journal of Mechanical and Mechatronics Engineering*, Published, Volume 13 (2019)
- **Yasaman Tohidi**, Rouzbeh Riazi, Shidvash Vakilipour, and Masoud Mohammadi “A Numerical Study on the Influence of CO₂ Dilution on Combustion Characteristics of a Turbulent Diffusion Flame”, *International Journal of Mechanical and Mechatronics Engineering*, Published, Volume 13 (2019)

Appendix A

Analytical Solution of Fully Developed Downward Laminar Two-Phase Flow in a Parallel Plate Channel

Based on the work of Saleh and Ormiston [11], an analytical solution has been obtained for fully-developed co-current laminar gas-liquid flow inside vertical parallel plate channels with symmetry condition applied at the channel centre line. The mass flow rates of the phases, the density and dynamic viscosity of both fluids, and the channel width are used as the input parameters.

For fully-developed conditions with constant properties, the momentum equations for the two phases reduce to the following:

$$\frac{d^2 U_L}{dy^2} = \frac{1}{\mu_L} \left(\frac{dP}{dx} - \rho_L g \right) \quad (\text{A.1})$$

and

$$\frac{d^2 U_M}{dy^2} = \frac{1}{\mu_M} \left(\frac{dP}{dx} - \rho_M g \right) \quad (\text{A.2})$$

Eq. (A.1) is integrated twice with respect to y for the limits $y = 0$ to $y = \delta_{\text{in}}$. Similarly, Eq. (A.2), is integrated twice for the limits $y = \delta_{\text{in}}$ to $y = H$. The resulting expressions for the velocities are:

$$U_L = \frac{1}{2\mu_L} \left(\frac{dP}{dx} - \rho_L g \right) y^2 + C_1 y + C_2 \quad \text{for } 0 \leq y \leq \delta_{\text{in}} \quad (\text{A.3})$$

$$U_M = \frac{1}{2\mu_M} \left(\frac{dP}{dx} - \rho_M g \right) y^2 + C_3 y + C_4 \quad \text{for } \delta_{\text{in}} \leq y \leq H \quad (\text{A.4})$$

The constants of integration in Eqs. (A.3) and (A.4) are determined by applying no-slip boundary condition at the wall ($y=0$), continuity of velocity and shear stress at the interface ($y = \delta$), and symmetry at the channel centre line ($y = H$). The symmetry condition at the centre line is the

Appendix A. Analytical Solution of Fully Developed Downward Laminar Two-Phase Flow in a Parallel Plate Channel

difference between this derivation and that in [111]. The constants of integration are obtained as follows:

$$C_1 = \left(\frac{-H}{\mu_L} \right) \frac{dP}{dx} + \left[\frac{1}{\mu_L} \left((\rho_L - \rho_M) \delta_{in} + \rho_M H \right) \right] g \quad (\text{A.5})$$

$$C_2 = 0 \quad (\text{A.6})$$

$$C_3 = \left(\frac{-H}{\mu_M} \right) \frac{dP}{dx} + \left(\frac{\rho_M H}{\mu_M} \right) g \quad (\text{A.7})$$

$$C_4 = \left[D \left(\frac{1}{\mu_L} - \frac{1}{\mu_M} \right) \right] \frac{dP}{dx} + \left[\frac{\delta_{in}^2 E}{2} + H \rho_M \delta_{in} \left(\frac{1}{\mu_L} - \frac{1}{\mu_M} \right) \right] g \quad (\text{A.8})$$

and

$$D = \frac{\delta_{in}^2}{2} - H \delta_{in} \quad (\text{A.9})$$

$$E = \frac{\rho_L}{\mu_L} - \frac{\rho_M}{\mu_M} - \frac{2\rho_M}{\mu_L} \quad (\text{A.10})$$

$$F = \frac{1}{6\mu_M} (H^3 - \delta_{in}^3) \quad (\text{A.11})$$

$$R = \frac{1}{2\mu_M} (H^2 - \delta_{in}^2) \quad (\text{A.12})$$

The velocity profiles can be integrated to obtain the liquid and mixture mass flow rates per unit depth of the channel:

$$\dot{m}'_L = \int_0^{\delta_{in}} \rho_L U_L dy = \rho_L C_5 \frac{dP}{dx} + \rho_L C_6 \quad (\text{A.13})$$

$$\dot{m}'_M = \int_{\delta_{in}}^H \rho_M U_M dy = \rho_M C_7 \frac{dP}{dx} + \rho_M C_8 \quad (\text{A.14})$$

where

$$C_5 = \frac{\delta_{in}^2}{6\mu_L} (\delta_{in} - 3H) \quad (\text{A.15})$$

$$C_6 = \left(\frac{\delta_{in}^2}{6\mu_L} \left(\delta_{in} \rho_L \left(2 - 3 \frac{\rho_M}{\rho_L} \right) + 3 \rho_M H \right) \right) g \quad (\text{A.16})$$

$$C_7 = F - HR + \left(D \left(\frac{1}{\mu_L} - \frac{1}{\mu_M} \right) \right) (H - \delta_{in}) \quad (\text{A.17})$$

Appendix A. Analytical Solution of Fully Developed Downward Laminar Two-Phase Flow in a Parallel Plate Channel

$$C_8 = \left(-\rho_M F + \rho_M H R + \left(\frac{\delta_{in}^2 E}{2} + H \rho_M \delta_{in} \left(\frac{1}{\mu_L} - \frac{1}{\mu_M} \right) \right) (H - \delta_{in}) \right) g \quad (A.18)$$

Given $\dot{m}'_L$ and $\dot{m}'_M$, Eqs. (A.13) and (A.14) can each be solved for pressure gradient, $\frac{dP}{dx}$. An equation for the film thickness, δ_{in} , can then be formed by equating the two equations for pressure gradient. After solving for δ_{in} , the pressure gradient is determined using either Eq. (A.13) or Eq. (A.14). Finally, Eqs. (A.1) and (A.2) are used to determine liquid and mixture velocity profiles, respectively.

Appendix B

Excess moisture condensation (EMC) model

The air is considered supersaturated when the amount of water vapour in the air exceeds the amount at the equilibrium condition. For the supersaturated state, the creation of liquid droplets in the mixture may occur due to either homogeneous or heterogeneous nucleation. In the presence of aerosols like dust and pollutants, the water vapour molecules can accumulate on the surface of aerosol particles, and heterogeneous nucleation occurs. In clean air, the water vapour molecules can merge to form a droplet; however, in the absence of aerosol particles, the droplet size is small and quickly evaporates [112]. So, no phase change occurs in the mixture unless the amount of water vapour is higher than a critical value resulting in the formation of large droplets and eventually the condensation of water vapour in the mixture. Carey [113] studied the non-equilibrium condition, referred to as the metastable state, in which the water vapour is in a supersaturation condition but no condensation occurs. He presented the following formula for homogeneous nucleation to calculate the critical partial pressure of water vapor as a supersaturation limit of the system.

$$SR = \frac{(P_{SSL})_v}{(P_{sat})_v} = \exp\left(\frac{E^* (-\ln J^*)^{0.5}}{2 (E^*)^{0.5} + (-\ln J^*)^{1.5}}\right)^{0.5} \quad (B.1)$$

where

$$J^* = \frac{10^6 M \rho_L}{N_A} \left(\frac{\pi M}{2 \sigma N_A}\right)^{0.5} \left[\frac{R T}{P_{sat}}\right] \quad (B.2)$$

and

$$E^* = \frac{16 \pi \sigma^3}{3 \rho_L^2 k_B R^2 T^3} \quad (B.3)$$

The surface tension of droplets, σ , is calculated using the formula presented in [107]. It is noted that Eq. (B.1) is valid only if dust particles and surface imperfections, which can act as nucleation sites, are not introduced to the system. The pressure ratio, SR, has been calculated explicitly using Eq. (B.1) for one of the cases studied in this work, W8, defined in Table 5.2, and the value was between 2.3 and 2.8. Therefore, in extremely clean air, the relative humidity could be between

230% and 280%. Because it is difficult to avoid the presence of the nucleation sites, the evaporation process can be initiated by heterogeneous nucleation in significantly smaller pressure ratios, and the relative humidity hardly exceeds 100%.

In the present study, the excess moisture condensation model is proposed as a novel method to deal with the effects of supersaturation in the system. In order to utilize this model, source terms $\dot{S}_C'''$, $\dot{S}_T'''$, and $\dot{S}_W'''$ are added to the continuity, energy, and gas species equations, respectively. The term $\dot{S}_C'''$ removes the excess mixture from the system. Eq. (B.4) is used as an initial guess for $\dot{S}_C'''$.

$$(\dot{S}_C''')_P = \frac{(a_P^{w,w})^{\text{old}}}{\nabla_P} \left(\frac{W_{\text{sat}}}{W_P^{\text{old}}} - 1 \right) \quad (\text{B.4})$$

Where $(a_P^{w,w})^{\text{old}}$ is the most recent value of the diagonal coefficient in the air mass fraction discretized equation. The value is updated in every iteration during the simulation using:

$$(\dot{S}_C''')_P^{\text{new}} = (\dot{S}_C''')_P^{\text{old}} + \alpha \frac{(a_P^{w,w})^{\text{old}}}{\nabla_P} (W_{\text{sat}} - W_P^{\text{old}}) \quad (\text{B.5})$$

α is a relaxation factor and set to be 0.002 in the present work. The mixture continuity mass sink removes both steam and air, so the air must be added back into the CV. The adding of air is accomplished using a source term $(\dot{S}_W''')$ in the gas species equation:

$$(\dot{S}_W''')_P = (\dot{S}_C''')_P W_P \quad (\text{B.6})$$

The effects on the energy balance are accounted for by using $\dot{S}_T'''$:

$$(\dot{S}_T''')_P = (\dot{S}_C''')_P (C_P)_P T_P - (\dot{S}_C''')_P (1 - W_P) (h_{fg})_P \quad (\text{B.7})$$

The first term on the right hand side of Eq. (B.7) compensates for the effect of sensible energy transported by the removed mixture. The second term on the right hand side accounts for the condensation of the excess moisture. The terms $\dot{S}_C'''$, $\dot{S}_T'''$, and $\dot{S}_W'''$ are set to zero for the control volumes where the relative humidity is less than 101%. At the end of the simulation, all control volumes where the EMC model is applied will be at saturation ($\phi \approx 100\%$). Therefore, the EMC model keeps a part of the domain at saturation where needed and leaves the rest under saturation as naturally predicted by the model equations.

Appendix C

Interfacial salt-water temperature function

A correlation based on the experimental data in [114] is used as the equilibrium condition. In equation (C.1), the interfacial salt-water temperature is defined as a function of vapour temperature and salinity.

$$T = T_v + \frac{S T_v^2}{13832} \left[1 + 0.001373 T_v - 0.00272 S^{0.5} T_v + 17.86 S - 0.0152 S T_v \left(\frac{T_v - 225.9}{T_v - 236} \right) - \frac{2583 S (1 - S)}{T_v} \right] \quad (\text{C.1})$$

where the validity ranges are $273.15 \leq T_v \leq 473.15$ K and $0 \leq S \leq 0.12$ kg/kg. The vapour temperature, T_v , is the saturation temperature, which is calculated based on the saturation vapour pressure at the interface [96].

Appendix D

Elliptic Model Coefficients in Algebraic Transport Equations

D.1 Continuity Equation coefficients

The coefficients of Equation (4.65) are:

$$a_{\text{P}}^{c,u} = \rho_e A_e n_{xe} \mathcal{W}_e - \rho_w A_w n_{xw} (1 - \mathcal{W}_w) + \rho_n A_n n_{xn} \mathcal{W}_n - \rho_s A_s n_{xs} (1 - \mathcal{W}_s) \quad (\text{D.1})$$

$$a_{\text{E}}^{c,u} = \rho_e A_e n_{xe} (1 - \mathcal{W}_e) \quad (\text{D.2})$$

$$a_{\text{W}}^{c,u} = -\rho_w A_w n_{xw} \mathcal{W}_w \quad (\text{D.3})$$

$$a_{\text{N}}^{c,u} = \rho_n A_n n_{xn} (1 - \mathcal{W}_n) \quad (\text{D.4})$$

$$a_{\text{S}}^{c,u} = -\rho_s A_s n_{xs} \mathcal{W}_s \quad (\text{D.5})$$

$$a_{\text{P}}^{c,v} = \rho_e A_e n_{ye} \mathcal{W}_e - \rho_w A_w n_{yw} (1 - \mathcal{W}_w) + \rho_n A_n n_{yn} \mathcal{W}_n - \rho_s A_s n_{ys} (1 - \mathcal{W}_s) \quad (\text{D.6})$$

$$a_{\text{E}}^{c,v} = \rho_e A_e n_{ye} (1 - \mathcal{W}_e) \quad (\text{D.7})$$

$$a_{\text{W}}^{c,v} = -\rho_w A_w n_{yw} \mathcal{W}_w \quad (\text{D.8})$$

$$a_N^{c,v} = \rho_n A_n n_{yn} (1 - \mathcal{W}_n) \quad (\text{D.9})$$

$$a_S^{c,v} = -\rho_s A_s n_{ys} \mathcal{W}_s \quad (\text{D.10})$$

$$\begin{aligned} a_P^{c,p} = & \rho_e A_e \hat{d}_e^u n_{xe} \left[\frac{\mathcal{Y}_{t,e}}{(ds)_e} + \frac{\mathcal{Y}_{s,e}}{(dt)_e} (C_{ne1} - C_{se4}) \right] + \rho_w A_w \hat{d}_w^u n_{xw} \left[\frac{\mathcal{Y}_{t,w}}{(ds)_w} - \frac{\mathcal{Y}_{s,w}}{(dt)_w} (C_{nw2} - C_{sw3}) \right] \\ & - \rho_n A_n \hat{d}_n^u n_{xn} \left[\frac{\mathcal{Y}_{s,n}}{(dt)_n} + \frac{\mathcal{Y}_{t,n}}{(ds)_n} (C_{ne1} - C_{nw2}) \right] - \rho_s A_s \hat{d}_s^u n_{xs} \left[\frac{\mathcal{Y}_{s,s}}{(dt)_s} - \frac{\mathcal{Y}_{t,s}}{(ds)_s} (C_{se4} - C_{sw3}) \right] \\ & - \rho_e A_e \hat{d}_e^v n_{ye} \left[\frac{\mathcal{X}_{t,e}}{(ds)_e} + \frac{\mathcal{X}_{s,e}}{(dt)_e} (C_{ne1} - C_{se4}) \right] - \rho_w A_w \hat{d}_w^v n_{yw} \left[\frac{\mathcal{X}_{t,w}}{(ds)_w} - \frac{\mathcal{X}_{s,w}}{(dt)_w} (C_{nw2} - C_{sw3}) \right] \\ & + \rho_n A_n \hat{d}_n^v n_{yn} \left[\frac{\mathcal{X}_{s,n}}{(dt)_n} + \frac{\mathcal{X}_{t,n}}{(ds)_n} (C_{ne1} - C_{nw2}) \right] + \rho_s A_s \hat{d}_s^v n_{ys} \left[\frac{\mathcal{X}_{s,s}}{(dt)_s} - \frac{\mathcal{X}_{t,s}}{(ds)_s} (C_{se4} - C_{sw3}) \right] \end{aligned} \quad (\text{D.11})$$

$$\begin{aligned} a_E^{c,p} = & -\rho_e A_e \left(\hat{d}_e^u n_{xe} \frac{\mathcal{Y}_{t,e}}{(ds)_e} - \hat{d}_e^v n_{ye} \frac{\mathcal{X}_{t,e}}{(ds)_e} \right) - \rho_n A_n \left(\hat{d}_n^u n_{xn} \frac{\mathcal{Y}_{t,n}}{(ds)_n} - \hat{d}_n^v n_{yn} \frac{\mathcal{X}_{t,n}}{(ds)_n} \right) C_{ne2} \\ & + \rho_s A_s \left(\hat{d}_s^u n_{xs} \frac{\mathcal{Y}_{t,s}}{(ds)_s} - \hat{d}_s^v n_{ys} \frac{\mathcal{X}_{t,s}}{(ds)_s} \right) C_{se3} + \rho_e A_e \left(\hat{d}_e^u n_{xe} \frac{\mathcal{Y}_{s,e}}{(dt)_e} - \hat{d}_e^v n_{ye} \frac{\mathcal{X}_{s,e}}{(dt)_e} \right) (C_{ne2} - C_{se3}) \end{aligned} \quad (\text{D.12})$$

$$\begin{aligned} a_W^{c,p} = & -\rho_w A_w \left(\hat{d}_w^u n_{xw} \frac{\mathcal{Y}_{t,w}}{(ds)_w} - \hat{d}_w^v n_{yw} \frac{\mathcal{X}_{t,w}}{(ds)_w} \right) + \rho_n A_n \left(\hat{d}_n^u n_{xn} \frac{\mathcal{Y}_{t,n}}{(ds)_n} - \hat{d}_n^v n_{yn} \frac{\mathcal{X}_{t,n}}{(ds)_n} \right) C_{nw1} \\ & - \rho_s A_s \left(\hat{d}_s^u n_{xs} \frac{\mathcal{Y}_{t,s}}{(ds)_s} - \hat{d}_s^v n_{ys} \frac{\mathcal{X}_{t,s}}{(ds)_s} \right) C_{sw4} + \rho_w A_w \left(\hat{d}_w^u n_{xw} \frac{\mathcal{Y}_{s,w}}{(dt)_w} - \hat{d}_w^v n_{yw} \frac{\mathcal{X}_{s,w}}{(dt)_w} \right) (C_{sw4} - C_{nw1}) \end{aligned} \quad (\text{D.13})$$

$$\begin{aligned} a_N^{c,p} = & \rho_n A_n \left(\hat{d}_n^u n_{xn} \frac{\mathcal{Y}_{s,n}}{(dt)_n} - \hat{d}_n^v n_{yn} \frac{\mathcal{X}_{s,n}}{(dt)_n} \right) + \rho_e A_e \left(\hat{d}_e^u n_{xe} \frac{\mathcal{Y}_{s,e}}{(dt)_e} - \hat{d}_e^v n_{ye} \frac{\mathcal{X}_{s,e}}{(dt)_e} \right) C_{ne4} \\ & - \rho_w A_w \left(\hat{d}_w^u n_{xw} \frac{\mathcal{Y}_{s,w}}{(dt)_w} - \hat{d}_w^v n_{yw} \frac{\mathcal{X}_{s,w}}{(dt)_w} \right) C_{nw3} - \rho_n A_n \left(\hat{d}_n^u n_{xn} \frac{\mathcal{Y}_{t,n}}{(ds)_n} - \hat{d}_n^v n_{yn} \frac{\mathcal{X}_{t,n}}{(ds)_n} \right) (C_{ne4} - C_{nw3}) \end{aligned} \quad (\text{D.14})$$

$$\begin{aligned} a_S^{c,p} = & \rho_s A_s \left(\hat{d}_s^u n_{xs} \frac{\mathcal{Y}_{s,s}}{(dt)_s} - \hat{d}_s^v n_{ys} \frac{\mathcal{X}_{s,s}}{(dt)_s} \right) - \rho_e A_e \left(\hat{d}_e^u n_{xe} \frac{\mathcal{Y}_{s,e}}{(dt)_e} - \hat{d}_e^v n_{ye} \frac{\mathcal{X}_{s,e}}{(dt)_e} \right) C_{se1} \\ & + \rho_w A_w \left(\hat{d}_w^u n_{xw} \frac{\mathcal{Y}_{s,w}}{(dt)_w} - \hat{d}_w^v n_{yw} \frac{\mathcal{X}_{s,w}}{(dt)_w} \right) C_{sw2} + \rho_s A_s \left(\hat{d}_s^u n_{xs} \frac{\mathcal{Y}_{t,s}}{(ds)_s} - \hat{d}_s^v n_{ys} \frac{\mathcal{X}_{t,s}}{(ds)_s} \right) (C_{se1} - C_{sw2}) \end{aligned} \quad (\text{D.15})$$

$$a_{\text{NE}}^{c,p} = \left(\rho_e A_e \hat{d}_e^u n_{xe} \frac{\mathcal{Y}_{s,e}}{(dt)_e} - \rho_e A_e \hat{d}_e^v n_{ye} \frac{\mathcal{X}_{s,e}}{(dt)_e} - \rho_n A_n \hat{d}_n^u n_{xn} \frac{\mathcal{Y}_{t,n}}{(ds)_n} + \rho_n A_n \hat{d}_n^v n_{yn} \frac{\mathcal{X}_{t,n}}{(ds)_n} \right) C_{ne3} \quad (\text{D.16})$$

$$a_{\text{NW}}^{c,p} = - \left(\rho_w A_w \hat{d}_w^u n_{xw} \frac{\mathcal{Y}_{s,w}}{(dt)_w} - \rho_w A_w \hat{d}_w^v n_{yw} \frac{\mathcal{X}_{s,w}}{(dt)_w} - \rho_n A_n \hat{d}_n^u n_{xn} \frac{\mathcal{Y}_{t,n}}{(ds)_n} + \rho_n A_n \hat{d}_n^v n_{yn} \frac{\mathcal{X}_{t,n}}{(ds)_n} \right) C_{nw4} \quad (\text{D.17})$$

$$a_{\text{SE}}^{c,p} = - \left(\rho_e A_e \hat{d}_e^u n_{xe} \frac{\mathcal{Y}_{s,e}}{(dt)_e} - \rho_e A_e \hat{d}_e^v n_{ye} \frac{\mathcal{X}_{s,e}}{(dt)_e} - \rho_s A_s \hat{d}_s^u n_{xs} \frac{\mathcal{Y}_{t,s}}{(ds)_s} + \rho_s A_s \hat{d}_s^v n_{ys} \frac{\mathcal{X}_{t,s}}{(ds)_s} \right) C_{se2} \quad (\text{D.18})$$

$$a_{\text{SW}}^{c,p} = \left(\rho_w A_w \hat{d}_w^u n_{xw} \frac{\mathcal{Y}_{s,w}}{(dt)_w} - \rho_w A_w \hat{d}_w^v n_{yw} \frac{\mathcal{X}_{s,w}}{(dt)_w} - \rho_s A_s \hat{d}_s^u n_{xs} \frac{\mathcal{Y}_{t,s}}{(ds)_s} + \rho_s A_s \hat{d}_s^v n_{ys} \frac{\mathcal{X}_{t,s}}{(ds)_s} \right) C_{sw1} \quad (\text{D.19})$$

$$b_{\text{P}}^c = -\rho_e A_e (n_{xe} \tilde{b}_e^u + n_{ye} \tilde{b}_e^v) + \rho_w A_w (n_{xw} \tilde{b}_w^u + n_{yw} \tilde{b}_w^v) - \rho_n A_n (n_{xn} \tilde{b}_n^u + n_{yn} \tilde{b}_n^v) + \rho_s A_s (n_{xs} \tilde{b}_s^u + n_{ys} \tilde{b}_s^v) \quad (\text{D.20})$$

D.2 Liquid Phase x -momentum Equation

$$\begin{aligned} a_{\text{P}}^{u,u} = & \left(\frac{\rho_{\text{P}} \mathcal{V}_{\text{P}}}{\Delta t} \right) + (0.5 + \alpha_e) \dot{m}_e - (0.5 - \alpha_w) \dot{m}_w + (0.5 + \alpha_n) \dot{m}_n - (0.5 - \alpha_s) \dot{m}_s \\ & + \frac{D_e^u \beta_e}{\hat{n}_e \cdot \hat{s}_e} + \frac{D_w^u \beta_w}{\hat{n}_w \cdot \hat{s}_w} + \frac{D_n^u \beta_n}{\hat{n}_n \cdot \hat{t}_n} + \frac{D_s^u \beta_s}{\hat{n}_s \cdot \hat{t}_s} + D_e^u \beta_e \gamma_{x,e} (C_{ne1} - C_{se4}) \\ & - D_w^u \beta_w \gamma_{x,w} (C_{nw2} - C_{sw3}) + D_n^u \beta_n \gamma_{y,n} (C_{ne1} - C_{nw2}) - D_s^u \beta_s \gamma_{y,s} (C_{se4} - C_{sw3}) \end{aligned} \quad (\text{D.21})$$

$$\begin{aligned} a_{\text{E}}^{u,u} = & (0.5 - \alpha_e) \dot{m}_e - \frac{D_e^u \beta_e}{\hat{n}_e \cdot \hat{s}_e} + D_n^u \beta_n \gamma_{y,n} C_{ne2} - D_s^u \beta_s \gamma_{y,s} C_{se3} \\ & + D_e^u \beta_e \gamma_{x,e} (C_{ne2} - C_{se3}) \end{aligned} \quad (\text{D.22})$$

$$a_W^{u,u} = -(0.5 + \alpha_w) \dot{m}_w - \frac{D_w^u \beta_w}{\hat{n}_w \cdot \hat{s}_w} - D_n^u \beta_n \gamma_{y,n} C_{nw1} + D_s^u \beta_s \gamma_{y,s} C_{sw4} - D_w^u \beta_w \gamma_{x,w} (C_{nw1} - C_{sw4}) \quad (D.23)$$

$$a_N^{u,u} = (0.5 - \alpha_n) \dot{m}_n - \frac{D_n^u \beta_n}{\hat{n}_n \cdot \hat{t}_n} + D_e^u \beta_e \gamma_{x,e} C_{ne4} - D_w^u \beta_w \gamma_{x,w} C_{nw3} + D_n^u \beta_n \gamma_{y,n} (C_{ne4} - C_{nw3}) \quad (D.24)$$

$$a_S^{u,u} = -(0.5 + \alpha_s) \dot{m}_s - \frac{D_s^u \beta_s}{\hat{n}_s \cdot \hat{t}_s} - D_e^u \beta_e \gamma_{x,e} C_{se1} + D_w^u \beta_w \gamma_{x,w} C_{sw2} - D_s^u \beta_s \gamma_{y,s} (C_{se1} - C_{sw2}) \quad (D.25)$$

$$a_{NE}^{u,u} = (D_e^u \beta_e \gamma_{x,e} + D_n^u \beta_n \gamma_{y,n}) C_{ne3} \quad (D.26)$$

$$a_{NW}^{u,u} = -(D_w^u \beta_w \gamma_{x,w} + D_n^u \beta_n \gamma_{y,n}) C_{nw4} \quad (D.27)$$

$$a_{SE}^{u,u} = -(D_e^u \beta_e \gamma_{x,e} + D_s^u \beta_s \gamma_{y,s}) C_{se2} \quad (D.28)$$

$$a_{SW}^{u,u} = (D_w^u \beta_w \gamma_{x,w} + D_s^u \beta_s \gamma_{y,s}) C_{sw1} \quad (D.29)$$

where,

$$D_e^u = \frac{\mu_e A_e}{(ds)_e} \quad D_w^u = \frac{\mu_w A_w}{(ds)_w} \quad D_n^u = \frac{\mu_n A_n}{(dt)_n} \quad D_s^u = \frac{\mu_s A_s}{(dt)_s} \quad (D.30)$$

$$\gamma_{x,f} = \frac{(ds)_f \hat{t}_f \cdot \hat{s}_f}{(dt)_f \hat{n}_f \cdot \hat{s}_f} \quad \gamma_{y,f} = \frac{(dt)_f \hat{t}_f \cdot \hat{s}_f}{(ds)_f \hat{n}_f \cdot \hat{t}_f} \quad (D.31)$$

The pressure coefficients of main node ($a_P^{u,p}$) and its four neighbours ($a_{NB4}^{u,p}$) are derived as follows:

$$a_P^{u,p} = \bar{V}_P \frac{\mathcal{Y}_{t,P}}{(ds)_P} (\mathcal{W}_e - 1 + \mathcal{W}_w) - \bar{V}_P \frac{\mathcal{Y}_{s,P}}{(dt)_P} (\mathcal{W}_n - 1 + \mathcal{W}_s) \quad (D.32)$$

$$a_E^{u,p} = \bar{V}_P \frac{\mathcal{Y}_{t,P}}{(ds)_P} (1 - \mathcal{W}_e) \quad (D.33)$$

$$a_W^{u,p} = -\bar{V}_P \frac{\mathcal{Y}_{t,P}}{(ds)_P} \mathcal{W}_w \quad (D.34)$$

$$a_N^{u,p} = -\bar{V}_P \frac{\mathcal{Y}_{s,P}}{(dt)_P} (1 - \mathcal{W}_n) \quad (D.35)$$

$$a_S^{u,p} = \bar{V}_P \frac{\mathcal{Y}_{s,P}}{(dt)_P} \mathcal{W}_s \quad (D.36)$$

The right hand side of Equation (4.78) is:

$$b_P^u = \left(\frac{\rho_P \bar{V}_P}{\Delta t} \right) U_P^o + \rho_P g_x \bar{V}_P \quad (D.37)$$

D.3 Liquid Phase y-momentum Equation

The coefficients of V-velocity of the main node and its neighbours are analogous to those of the U-momentum equation:

$$a_P^{v,v} = a_P^{u,u} \quad a_{NB}^{v,v} = a_{NB}^{u,u} \quad (D.38)$$

Note that D_f^u changes to D_f^v and $D_f^v = D_f^u$ (Equation (D.30)). The other coefficients are as follows:

$$a_P^{v,p} = \bar{V}_P \frac{\mathcal{X}_{s,P}}{(dt)_P} (\mathcal{W}_n - 1 + \mathcal{W}_s) - \bar{V}_P \frac{\mathcal{X}_{t,P}}{(ds)_P} (\mathcal{W}_e - 1 + \mathcal{W}_w) \quad (D.39)$$

$$a_E^{v,p} = -\bar{V}_P \frac{\mathcal{X}_{t,P}}{(ds)_P} (1 - \mathcal{W}_e) \quad (D.40)$$

$$a_W^{v,p} = \mathcal{V}_P \frac{\mathcal{X}_{t,P}}{(ds)_P} \mathcal{W}_w \quad (\text{D.41})$$

$$a_N^{v,p} = \mathcal{V}_P \frac{\mathcal{X}_{s,P}}{(dt)_P} (1 - \mathcal{W}_n) \quad (\text{D.42})$$

$$a_S^{v,p} = -\mathcal{V}_P \frac{\mathcal{X}_{s,P}}{(dt)_P} \mathcal{W}_s \quad (\text{D.43})$$

$$b_P^v = \left(\frac{\rho_P \mathcal{V}_P}{\Delta t} \right) V_P^o \quad (\text{D.44})$$

D.4 Liquid Phase Energy Equation

The derivation of $a_P^{t,t}$ and $a_{NB}^{t,t}$ is analogous to those for the U velocity coefficient in the x -momentum equation using k of μ in D_f coefficients and $\dot{m}C_p$ instead of $\dot{m}$.

$$D_e^t = \frac{k_e A_e}{(ds)_e} \quad D_w^t = \frac{k_w A_w}{(ds)_w} \quad D_n^t = \frac{k_n A_n}{(dt)_n} \quad D_s^t = \frac{k_s A_s}{(dt)_s} \quad (\text{D.45})$$

$$\begin{aligned} a_P^{t,W} = & (0.5 + \alpha_e) (\bar{h}_S - \bar{h}_W)_e \dot{m}_e - (0.5 - \alpha_w) (\bar{h}_S - \bar{h}_W)_w \dot{m}_w \\ & + (0.5 + \alpha_n) (\bar{h}_S - \bar{h}_W)_n \dot{m}_n - (0.5 - \alpha_s) (\bar{h}_S - \bar{h}_W)_s \dot{m}_s \\ & + \frac{\tilde{D}_e^t \beta_e}{\hat{n}_e \cdot \hat{s}_e} + \frac{\tilde{D}_w^t \beta_w}{\hat{n}_w \cdot \hat{s}_w} + \frac{\tilde{D}_n^t \beta_n}{\hat{n}_n \cdot \hat{t}_n} + \frac{\tilde{D}_s^t \beta_s}{\hat{n}_s \cdot \hat{t}_s} + \tilde{D}_e^t \beta_e \gamma_{x,e} (C_{ne1} - C_{se4}) \\ & - \tilde{D}_w^t \beta_w \gamma_{x,w} (C_{nw2} - C_{sw3}) + \tilde{D}_n^t \beta_n \gamma_{y,n} (C_{ne1} - C_{nw2}) - \tilde{D}_s^t \beta_s \gamma_{y,s} (C_{se4} - C_{sw3}) \end{aligned} \quad (\text{D.46})$$

$$\begin{aligned} a_E^{t,W} = & (0.5 - \alpha_e) (\bar{h}_S - \bar{h}_W)_e \dot{m}_e - \frac{\tilde{D}_e^t \beta_e}{\hat{n}_e \cdot \hat{s}_e} + \tilde{D}_n^t \beta_n \gamma_{y,n} C_{ne2} - \tilde{D}_s^t \beta_s \gamma_{y,s} C_{se3} \\ & + \tilde{D}_e^t \beta_e \gamma_{x,e} (C_{ne2} - C_{se3}) \end{aligned} \quad (\text{D.47})$$

$$a_W^{t,W} = -(0.5 + \alpha_w) (\bar{h}_S - \bar{h}_W)_w \dot{m}_w - \frac{\tilde{D}_w^t \beta_w}{\hat{n}_w \cdot \hat{s}_w} - \tilde{D}_n^t \beta_n \gamma_{y,n} C_{nw1} + \tilde{D}_s^t \beta_s \gamma_{y,s} C_{sw4} - \tilde{D}_w^t \beta_w \gamma_{x,w} (C_{nw1} - C_{sw4}) \quad (D.48)$$

$$a_N^{t,W} = (0.5 - \alpha_n) (\bar{h}_S - \bar{h}_W)_n \dot{m}_n - \frac{\tilde{D}_n^t \beta_n}{\hat{n}_n \cdot \hat{t}_n} + \tilde{D}_e^t \beta_e \gamma_{x,e} C_{ne4} - \tilde{D}_w^t \beta_w \gamma_{x,w} C_{nw3} + \tilde{D}_n^t \beta_n \gamma_{y,n} (C_{ne4} - C_{nw3}) \quad (D.49)$$

$$a_S^{t,W} = -(0.5 + \alpha_s) (\bar{h}_S - \bar{h}_W)_s \dot{m}_s - \frac{\tilde{D}_s^t \beta_s}{\hat{n}_s \cdot \hat{t}_s} - \tilde{D}_e^t \beta_e \gamma_{x,e} C_{se1} + \tilde{D}_w^t \beta_w \gamma_{x,w} C_{sw2} - \tilde{D}_s^t \beta_s \gamma_{y,s} (C_{se1} - C_{sw2}) \quad (D.50)$$

$$a_{NE}^{t,W} = (\tilde{D}_e^t \beta_e \gamma_{x,e} + \tilde{D}_n^t \beta_n \gamma_{y,n}) C_{ne3} \quad (D.51)$$

$$a_{SE}^{t,W} = -(\tilde{D}_e^t \beta_e \gamma_{x,e} + \tilde{D}_s^t \beta_s \gamma_{y,s}) C_{se2} \quad (D.52)$$

$$a_{NW}^{t,W} = -(\tilde{D}_w^t \beta_w \gamma_{x,w} + \tilde{D}_n^t \beta_n \gamma_{y,n}) C_{nw4} \quad (D.53)$$

$$a_{SW}^{t,W} = (\tilde{D}_w^t \beta_w \gamma_{x,w} + \tilde{D}_s^t \beta_s \gamma_{y,s}) C_{sw1} \quad (D.54)$$

where,

$$\begin{aligned} \tilde{D}_e^t &= \frac{\rho_e D_e^{AB} A_e (\bar{h}_S - \bar{h}_W)_e}{(ds)_e} & \tilde{D}_w^t &= \frac{\rho_w D_w^{AB} A_w (\bar{h}_S - \bar{h}_W)_w}{(ds)_w} \\ \tilde{D}_n^t &= \frac{\rho_n D_n^{AB} A_n (\bar{h}_S - \bar{h}_W)_n}{(dt)_n} & \tilde{D}_s^t &= \frac{\rho_s D_s^{AB} A_s (\bar{h}_S - \bar{h}_W)_s}{(dt)_s} \end{aligned} \quad (D.55)$$

$$b_P^t = \left(\frac{\rho_P C_{pP} \overline{V}_P}{\Delta t} \right) T_P^o \quad (\text{D.56})$$

Appendix E

Elliptic Model Coefficients in Interface Algebraic Equations

E.1 Normal Force Balance

The coefficients of Equation (4.99) are:

$$a_{iL,P}^{c,P} = 1 \quad (\text{E.1})$$

$$a_{iL,N}^{c,P} = -1 \quad (\text{E.2})$$

$$a_{iL,P}^{c,u} = -2 \mu_{iL,P} (n_{xn}^2 A_{x2} + n_{xn} n_{yn} A_{y2})_{iL,S} \quad (\text{E.3})$$

$$a_{iL,E}^{c,u} = -2 \mu_{iL,P} (n_{xn}^2 A_{x3} + n_{xn} n_{yn} A_{y3})_{iL,S} \quad (\text{E.4})$$

$$a_{iL,W}^{c,u} = -2 \mu_{iL,P} (n_{xn}^2 A_{x4} + n_{xn} n_{yn} A_{y4})_{iL,S} \quad (\text{E.5})$$

$$a_{iL,S}^{c,u} = -2 \mu_{iL,P} (n_{xn}^2 A_{x1} + n_{xn} n_{yn} A_{y1})_{iL,S} \quad (\text{E.6})$$

$$a_{iL,P}^{c,v} = -2 \mu_{iL,P} (n_{xn} n_{yn} A_{x2} + n_{yn}^2 A_{y2})_{iL,S} \quad (\text{E.7})$$

$$a_{iL,E}^{c,v} = -2 \mu_{iL,P} (n_{xn} n_{yn} A_{x3} + n_{yn}^2 A_{y3})_{iL,S} \quad (\text{E.8})$$

$$a_{iL,W}^{c,v} = -2 \mu_{iL,P} (n_{xn} n_{yn} A_{x4} + n_{yn}^2 A_{y4})_{iL,S} \quad (\text{E.9})$$

$$a_{iL,S}^{c,v} = -2 \mu_{iL,P} (n_{xn} n_{yn} A_{x1} + n_{yn}^2 A_{y1})_{iL,S} \quad (\text{E.10})$$

$$a_{iL,N}^{c,u} = 2 \mu_{iG,P} (n_{xs}^2 B_{x2} + n_{xs} n_{ys} B_{y2})_{iG,N} \quad (\text{E.11})$$

$$a_{iL,NE}^{c,u} = 2 \mu_{iG,P} (n_{xs}^2 B_{x3} + n_{xs} n_{ys} B_{y3})_{iG,N} \quad (\text{E.12})$$

$$a_{iL,NW}^{c,u} = 2 \mu_{iG,P} (n_{xs}^2 B_{x4} + n_{xs} n_{ys} B_{y4})_{iG,N} \quad (\text{E.13})$$

$$a_{iL,N}^{c,v} = 2 \mu_{iG,P} (n_{xs} n_{ys} B_{x2} + n_{ys}^2 B_{y2})_{iG,N} \quad (\text{E.14})$$

$$a_{iL,NE}^{c,v} = 2 \mu_{iG,P} (n_{xs} n_{ys} B_{x3} + n_{ys}^2 B_{y3})_{iG,N} \quad (\text{E.15})$$

$$a_{iL,NW}^{c,v} = 2 \mu_{iG,P} (n_{xs} n_{ys} B_{x4} + n_{ys}^2 B_{y4})_{iG,N} \quad (\text{E.16})$$

$$b_{iL,P}^c = -\sigma K - 2\mu_{iG,P} \left(n_{xs}^2 B_{x1} + n_{xs} n_{ys} B_{y1} \right)_{iG,N} U_{iG,N} - 2\mu_{iG,P} \left(n_{xs} n_{ys} B_{x1} + n_{ys}^2 B_{y1} \right)_{iG,N} V_{iG,N} \quad (\text{E.17})$$

E.2 Zero Pressure Gradient

The coefficients of Equation (4.101) are:

$$a_{iG,P}^{c,p} = \left(B_{x2} n_{xs} + B_{y2} n_{ys} \right)_{iG,N} \quad (\text{E.18})$$

$$a_{iG,N}^{c,p} = \left(B_{x1} n_{xs} + B_{y1} n_{ys} \right)_{iG,N} \quad (\text{E.19})$$

$$a_{iG,W}^{c,p} = \left(B_{x4} n_{xs} + B_{y4} n_{ys} \right)_{iG,N} \quad (\text{E.20})$$

$$a_{iG,E}^{c,p} = \left(B_{x3} n_{xs} + B_{y3} n_{ys} \right)_{iG,N} \quad (\text{E.21})$$

E.3 Tangential Force Balance

The coefficients of Equation (4.105) are:

$$a_{iG,P}^{u,u} = -\mu_{iG,P} \left(2n_{xs}s_{xs}B_{x2} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{y2} \right)_{iG,N} \quad (E.22)$$

$$a_{iG,E}^{u,u} = -\mu_{iG,P} \left(2n_{xs}s_{xs}B_{x3} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{y3} \right)_{iG,N} \quad (E.23)$$

$$a_{iG,W}^{u,u} = -\mu_{iG,P} \left(2n_{xs}s_{xs}B_{x4} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{y4} \right)_{iG,N} \quad (E.24)$$

$$a_{iG,N}^{u,u} = -\mu_{iG,P} \left(2n_{xs}s_{xs}B_{x1} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{y1} \right)_{iG,N} \quad (E.25)$$

$$a_{iG,P}^{u,v} = -\mu_{iG,P} \left(2n_{ys}s_{ys}B_{y2} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{x2} \right)_{iG,N} \quad (E.26)$$

$$a_{iG,E}^{u,v} = -\mu_{iG,P} \left(2n_{ys}s_{ys}B_{y3} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{x3} \right)_{iG,N} \quad (E.27)$$

$$a_{iG,W}^{u,v} = -\mu_{iG,P} \left(2n_{ys}s_{ys}B_{y4} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{x4} \right)_{iG,N} \quad (E.28)$$

$$a_{iG,N}^{u,v} = -\mu_{iG,P} \left(2n_{ys}s_{ys}B_{y1} + (n_{ys}s_{xs} + n_{xs}s_{ys})B_{x1} \right)_{iG,N} \quad (E.29)$$

$$a_{iG,S}^{u,u} = \mu_{iL,P} \left(2n_{xn}s_{xn}A_{x2} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{y2} \right)_{iL,S} \quad (E.30)$$

$$a_{iG,SE}^{u,u} = \mu_{iL,P} \left(2n_{xn}s_{xn}A_{x3} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{y3} \right)_{iL,S} \quad (E.31)$$

$$a_{iG,SW}^{u,u} = \mu_{iL,P} \left(2n_{xn}s_{xn}A_{x4} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{y4} \right)_{iL,S} \quad (E.32)$$

$$a_{iG,S}^{u,v} = \mu_{iL,P} \left(2n_{yn}s_{yn}A_{y2} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{x2} \right)_{iL,S} \quad (E.33)$$

$$a_{iG,SE}^{u,v} = \mu_{iL,P} \left(2n_{yn}s_{yn}A_{y3} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{x3} \right)_{iL,S} \quad (E.34)$$

$$a_{iG,SW}^{u,v} = \mu_{iL,P} \left(2n_{yn}s_{yn}A_{y4} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{x4} \right)_{iL,S} \quad (E.35)$$

$$b_{iG,P}^u = \frac{\partial \sigma}{\partial s} \Big|_{L,\text{intf}} - \mu_{iL,P} \left(2n_{xn}s_{xn}A_{x1} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{y1} \right)_{iL,S} U_{iL,S} - \mu_{iL,P} \left(2n_{yn}s_{yn}A_{y1} + (n_{yn}s_{xn} + n_{xn}s_{yn})A_{x1} \right)_{iL,S} V_{iL,S} \quad (E.36)$$

E.4 Tangential Velocity Equality

The coefficients of Equation (4.107) are:

$$a_{iL,P}^{u,u} = s_{xn}|_{iL,S} \quad (\text{E.37})$$

$$a_{iL,N}^{u,u} = -s_{xs}|_{iG,N} \quad (\text{E.38})$$

$$a_{iL,P}^{u,v} = s_{yn}|_{iL,S} \quad (\text{E.39})$$

$$a_{iL,N}^{u,v} = -s_{ys}|_{iG,N} \quad (\text{E.40})$$

E.5 Continuity of Mass at the Interface

The coefficients of Equation (4.109) are:

$$a_{iG,P}^{v,u} = (\rho A)_{iG,P}(n_{xs})_{iG,N} \quad (\text{E.41})$$

$$a_{iG,S}^{v,u} = -(\rho A)_{iL,P}(n_{xn})_{iL,S} \quad (\text{E.42})$$

$$a_{iG,P}^{v,v} = (\rho A)_{iG,P}(n_{ys})_{iG,N} \quad (\text{E.43})$$

$$a_{iG,S}^{v,v} = -(\rho A)_{iL,P}(n_{yn})_{iL,S} \quad (\text{E.44})$$

E.6 Continuity of Energy at the Interface

The coefficients of Equation (4.111) are:

$$a_{iL,P}^{v,u} = (\rho A)_{iL,P} (n_{xn})_{iL,S} \quad (E.45)$$

$$a_{iL,P}^{v,v} = (\rho A)_{iL,P} (n_{yn})_{iL,S} \quad (E.46)$$

$$a_{iL,P}^{v,t} = \frac{kA}{h_{fg}} \Big|_{iL,P} (A_{x2} n_{xn} + A_{y2} n_{yn})_{iL,S} \quad (E.47)$$

$$a_{iL,E}^{v,t} = \frac{kA}{h_{fg}} \Big|_{iL,P} (A_{x3} n_{xn} + A_{y3} n_{yn})_{iL,S} \quad (E.48)$$

$$a_{iL,W}^{v,t} = \frac{kA}{h_{fg}} \Big|_{iL,P} (A_{x4} n_{xn} + A_{y4} n_{yn})_{iL,S} \quad (E.49)$$

$$a_{iL,S}^{v,t} = \frac{kA}{h_{fg}} \Big|_{iL,P} (A_{x1} n_{xn} + A_{y1} n_{yn})_{iL,S} \quad (E.50)$$

$$a_{iL,N}^{v,t} = -\frac{kA}{h_{fg}} \Big|_{iG,P} (B_{x2} n_{xs} + B_{y2} n_{ys})_{iG,N} \quad (E.51)$$

$$a_{iL,NE}^{v,t} = -\frac{kA}{h_{fg}} \Big|_{iG,P} (B_{x3} n_{xs} + B_{y3} n_{ys})_{iG,N} \quad (E.52)$$

$$a_{iL,NW}^{v,t} = -\frac{kA}{h_{fg}} \Big|_{iG,P} (B_{x4} n_{xs} + B_{y4} n_{ys})_{iG,N} \quad (E.53)$$

$$b_{iL,P}^v = \frac{kA}{h_{fg}} \Big|_{iG,P} (B_{x1} n_{xs} + B_{y1} n_{ys})_{iG,N} T_{iG,N} \quad (E.54)$$

E.7 Equilibrium Condition at the Interface

The coefficients of Equation (4.113) are:

$$a_{iL,P}^{t,t} = 1 \quad (E.55)$$

$$a_{iL,P}^{t,w} = -\frac{\partial F}{\partial W_{iL}} \quad (E.56)$$

$$a_{iG,P}^{t,P} = -\frac{\partial F}{\partial P_{iG}} \quad (E.57)$$

$$a_{iG,P}^{t,w} = -\frac{\partial F}{\partial W_{iG}} \quad (E.58)$$

$$b_{iL,P}^t = T_{iL,P}^o - \frac{\partial F}{\partial W_{iL}} W_{iL}^o - \frac{\partial F}{\partial P_{iG}} P_{iG}^o - \frac{\partial F}{\partial W_{iG}} W_{iG}^o \quad (\text{E.59})$$

E.8 Temperature Equality at the Interface

The coefficients of Equation (4.114) are:

$$a_{iG,P}^{t,t} = 1 \quad (\text{E.60})$$

$$a_{iG,S}^{t,t} = -1 \quad (\text{E.61})$$

E.9 Impermeability of Gas

The coefficients of Equation 4.116 are:

$$\begin{aligned} a_{iG,P}^{w,w} = & -(\rho A D^{AB})_{iG,P} (n_{xn} B_{x2} + n_{yn} B_{y2})_{iG,N} \\ & + (\rho A U^o)_{iG,P} n_{xn}|_{iG,S} + (\rho A V^o)_{iG,P} n_{yn}|_{iG,N} \end{aligned} \quad (\text{E.62})$$

$$a_{iG,E}^{w,w} = -(\rho A D^{AB})_{iG,P} (n_{xn} B_{x3} + n_{yn} B_{y3})_{iG,N} \quad (\text{E.63})$$

$$a_{iG,W}^{w,w} = -(\rho A D^{AB})_{iG,P} (n_{xn} B_{x4} + n_{yn} B_{y4})_{iG,N} \quad (\text{E.64})$$

$$a_{iG,S}^{w,w} = -(\rho A D^{AB})_{iG,P} (n_{xn} B_{x1} + n_{yn} B_{y1})_{iG,N} \quad (\text{E.65})$$

$$a_{iG,P}^{w,u} = (\rho A)_{iG,P} n_{xn}|_{iG,N} (W^o)_{iG,P} \quad (\text{E.66})$$

$$a_{iG,P}^{w,v} = (\rho A)_{iG,P} n_{yn}|_{iG,N} (W^o)_{iG,P} \quad (\text{E.67})$$

$$b_{iG,P}^w = (\rho A U^o W^o)_{iG,P} n_{xn}|_{iG,N} + (\rho A V^o W^o)_{iG,P} n_{yn}|_{iG,N} \quad (\text{E.68})$$

E.10 Impermeability of Salt

The coefficients of Equation (4.118) are:

$$a_{iL,P}^{w,w} = -(\rho AD^{AB})_{iL,P} (n_{xn} A_{x2} + n_{yn} A_{y2})_{iL,S} + (\rho AU^o)_{iL,P} n_{xn}|_{iL,S} + (\rho AV^o)_{iL,P} n_{yn}|_{iL,S} \quad (E.69)$$

$$a_{iL,E}^{w,w} = -(\rho AD^{AB})_{iL,P} (n_{xn} A_{x3} + n_{yn} A_{y3})_{iL,S} \quad (E.70)$$

$$a_{iL,W}^{w,w} = -(\rho AD^{AB})_{iL,P} (n_{xn} A_{x4} + n_{yn} A_{y4})_{iL,S} \quad (E.71)$$

$$a_{iL,S}^{w,w} = -(\rho AD^{AB})_{iL,P} (n_{xn} A_{x1} + n_{yn} A_{y1})_{iL,S} \quad (E.72)$$

$$a_{iL,P}^{w,u} = (\rho A)_{iL,P} n_{xn}|_{iL,S} (W^o)_{iL,P} \quad (E.73)$$

$$a_{iL,P}^{w,v} = (\rho A)_{iL,P} n_{yn}|_{iL,S} (W^o)_{iL,P} \quad (E.74)$$

$$b_{iL,P}^w = (\rho AU^o W^o)_{iL,P} n_{xn}|_{iL,S} + (\rho AV^o W^o)_{iL,P} n_{yn}|_{iL,S} \quad (E.75)$$