

Technische Universität München
TUM School of Engineering and Design

Water Evaporation CFD Methods for Predicting the Dry-Out Time of Automotive Parts

JungHoon Lee

Vollständiger Abdruck der von der TUM School of Engineering and Design der Technischen Universität München zur Erlangung eines
Doktors der Ingenieurwissenschaften (Dr.-Ing.)
genehmigten Dissertation.

Vorsitz: Prof. Dr.-Ing. Klaus Drechsler

Prüfende der Dissertation:

1. Prof. Dr.-Ing. Harald Klein
2. Prof. Dr.-Ing. Helge Stein

Die Dissertation wurde am 03.03.2025 bei der Technischen Universität München eingereicht
und durch die TUM School of Engineering and Design am 10.06.2025 angenommen.

Soli Deo Gloria

Acknowledgements

First of all, I would like to express my deepest gratitude to my wife EunKyung and my daughter Aurum, who give unlimited supports to me both physically and spiritually. I also want to thank my family in Daegu and my family in Seoul for their full material and emotional supports.

Secondly, I am most sincerely grateful to my supervisor Dr. Dirk Bäder at AUDI AG, Prof. Dr.-Ing. Harald Klein and Dr.-Ing. Sebastian Rehfeldt at Technical University of Munich (TUM) for their full support, advice and motivations. Also, I want to thank them for providing me such a great opportunity.

I also would like to thank to Dr. Almut Eisenträger and Dr. Isabel Michel and Dr. Jörg Kuhnert from Fraunhofer ITWM for their full technical support and academic license for the software MESHFREE provided by Fraunhofer ITWM and Fraunhofer SCAI to complete this work.

Furthermore, I must express my gratitude to Mrs. Kerstin Meißner and the entire team members of “Corrosion/water protection, functional development of the complete vehicle” department in AUDI AG for their technical advice and kindness.

Lastly, but not least, I want to express my deepest gratitude to God, my Lord, who has led my life until now and will lead it to the End.

Publications

Parts of the work presented in this thesis have been published in the following peer-reviewed journal articles

Lee, J.; Bäder, D.; Rehfeldt, S.; Eisenträger, A.; Kuhnert, J.; Michel, I.; Suchde, P.; Klein, H.: *Modeling evaporation with a meshfree collocation approach*. Computational Particle Mechanics 10 (2023), pp. 1989–2007. DOI: 10.1007/s40571-023-00602-0.

Lee, J.; Bäder, D.; Rehfeldt, S.; Klein, H.: *Water Evaporation CFD Method with the Meshfree Volume-Volume-Coupling Approach for Wet Automotive Component Dry-Out Time Prediction*. International Journal of Automotive Engineering 15.1 (2024), pp. 58–65. DOI: 10.20485/jsaeijae.15.1_58.

and following conference articles

Lee, J.; Bäder, D.; Rehfeldt, S.; Eisenträger, A.; Kuhnert, J.; Michel, I.; Klein, H.: *Two-phase MESHFREE simulations with mass transfer model for free water surface evaporation*. 15th World Congress on Computational Mechanics & 8th Asian Pacific Congress on Computational Mechanics. International Association for Computational Mechanics. July 2022.

Lee, J.; Bäder, D.; Rehfeldt, S.; Eisenträger, A.; Kuhnert, J.; Michel, I.; Klein, H.: *Two-phase water evaporation MESHFREE CFD method for wet automotive component dry-out time prediction*. SIMVEC (SIMulation in VEHicle) 2022. VDI Wissensforum. Nov. 2022.

Lee, J.; Bäder, D.; Rehfeldt, S.; Klein, H.: *VOF-based concentration-gradient-driven mass transfer model for water evaporation*. 10th OpenFOAM Conference. ESI Group. Nov. 2022.

Lee, J.; Bäder, D.; Rehfeldt, S.; Klein, H.: *Dry-Out Time Prediction of Automotive Applications with Water Evaporation CFD using a Meshfree Collocation Approach*. NAFEMS International Multiphysics Conference. NAFEMS. Nov. 2023.

Lee, J.; Bäder, D.; Rehfeldt, S.; Klein, H.: *Water Evaporation CFD Method with a Meshfree Collocation Approach for Wet Automotive Component Dry-out time Prediction*. JSAE Autumn 2023. Society of Automotive Engineers of Japan. Oct. 2023.

Abstract

The goal of this doctoral project is to develop a robust CFD (Computational Fluid Dynamics) simulation method to resolve the water evaporation phenomenon and estimate the corresponding evaporation rate at the free surface region. With the calculated evaporation rate, the total dry-out time can be precisely approximated so that proper corrosion protection schemes on potentially wet automotive components can be applied. In this thesis, new methods to resolve the below-boiling point evaporation of water are introduced, which are developed using both mesh-based and meshless numerical methods. The developed methods are first validated with a series of experiments using relatively simple geometries under different ambient conditions. Here, measured and calculated evaporation rates are compared to analyze the performance of each method. Considering the performance and the applicability, the most promising method, specifically the method developed with the GFDM (Generalized Finite Difference Method) with the volume-volume-coupling, is deployed for the dry-out time validation with actual vehicle geometry applications. This application focuses on the automotive industry, where understanding and controlling water evaporation is crucial for preventing corrosion and ensuring component durability. Further, a typical exemplary case of the method's deployment is also showcased. Finally, the potential application of the newly developed method to a more complex and comprehensive vehicle geometry is demonstrated as an example of its further applications.

Contents

Nomenclature	XI
1 Introduction	1
1.1 Motivation and Objective	1
1.2 Thesis Outline	2
1.3 General Remarks	3
2 Literature Review	5
2.1 Numerical methods for CFD	5
2.2 Applications of CFD in automotive water management	6
2.3 CFD methods for evaporation physics	7
2.4 Experimental evaporation process measurement	10
3 Background theories and methodologies	13
3.1 Brief background physical theories	14
3.1.1 Theories of evaporation	14
3.1.2 Theories of localized corrosion	15
3.2 Computational Fluid Dynamics	17
3.3 Fundamental governing equations	17
3.4 Extension of governing equations	19
3.4.1 Turbulence equations	19
3.4.2 Species transport equation	19
3.5 Fluid modeling: single- and multi-phase	20
3.6 Modeling and Implementations in GFDM	20
3.6.1 Generalized Finite Difference Method	21
3.6.2 Single-phase approach for evaporation	36
3.6.3 Multi-phase approaches for evaporation	38
3.7 Modeling and Implementations in FVM	45
3.7.1 Finite Volume Method	45
3.7.2 Volume of Fluid (VoF) model	53
3.7.3 Multi-component mixture model	54
3.7.4 Mass transfer and thermal balance	55
3.7.5 Boundary conditions	57
4 Validation with a water vessel in a channel geometry	59
4.1 Experimental setup	59
4.2 Numerical simulation results	60
4.2.1 OpenFOAM results	63

4.2.2	MESHFREE single-phase results	69
4.2.3	MESHFREE multi-phase results	70
4.3	Validation results comparison and discussion	79
4.3.1	Runtime Comparison	79
4.3.2	Error Comparison	80
4.3.3	Overall discussion of various approaches	81
5	Validation and application to vehicle geometries	87
5.1	Sunroof channel geometry case for Vehicle A	87
5.1.1	Experiment setup	87
5.1.2	Numerical simulation results	89
5.2	Sunroof channel geometry case for Vehicle B	95
5.2.1	Application for different component design variations in develop- ment process	95
5.2.2	Experiment setup	97
5.2.3	Numerical simulation results	100
6	Further applications	103
6.1	Application to more sophisticated vehicle geometries	103
6.2	Application of the thermal effects of vehicle components	106
7	Conclusion	109
	List of Tables	111
	List of Figures	112
	Bibliography	117

Nomenclature

Symbols

$\boldsymbol{a}$	Acceleration	m/s^2
A	Area	m^2
B	Source term of linear system of algebraic equations	
$\mathcal{B}$	Source term vector	
$c^*, \mathbf{c}^*$	Numerical differential operator with wild-card	
c_v	Isochoric heat capacity	$\text{J}/(\text{kg K})$
c_p	Isobaric heat capacity	$\text{J}/(\text{kg K})$
$C_{1\varepsilon}, C_{2\varepsilon}, C_{3\varepsilon}$	Coefficients in k- ε model	
C_η	Coefficients in k- ε model	
D	Diffusivity	m^2/s
e	Error	
E	Specific total energy	J/kg
$\boldsymbol{F}$	Force	N
F	Mass flux	kg/s
$\boldsymbol{g}$	Gravitational body force	m/s^2
h	Smoothing length	m
Δh	Latent heat of evaporation	J/g
$\boldsymbol{I}$	Identity tensor	
k	Turbulent kinetic energy	m^2/s^2
L	Characteristic length	m
m	Mass	kg
$\dot{m}''$	Mass transfer rate (mass flux)	$\text{kg}/(\text{m}^2 \text{s})$
M	Molar mass	g/mol
$\dot{M}''$	Cell-wise mass transfer rate (mass flux)	$\text{kg}/(\text{m}^2 \text{s})$
$\mathcal{M}$	Solution matrix of system of linear algebraic equations	
$\boldsymbol{n}$	Surface normal unit vector	

N	Set of neighboring points in GFDM	
$NP, NP(t)$	Total number of points in domain in GFDM	
p	Pressure	Pa
P_{pr}	Turbulent production rate	
P_b	Turbulent buoyancy	
$\dot{q}''$	Heat flux	W/m ²
$r_{\min}$	Minimum search radius coefficient	
$r_{\max}$	Maximum search radius coefficient	
$\mathbf{S}$	Stress tensor	Pa
$\mathbf{S}_f$	Outward face area vector	m ²
S	Source term	Pa
$\mathbf{S}_{\text{solid}}$	Solid stress tensor	Pa
$\mathbf{S}_{\text{visc}}$	Viscous stress tensor	Pa
$\mathbf{S}_\sigma$	Volumetric surface tension force	N/m ³
t	Time	s
$\mathbf{t}$	Surface tangential unit vector	
Δt	Time step size	s
u	Velocity component	m/s
$\mathbf{v}$	Velocity	m/s
v	Velocity component	m/s
V	Volume	m ³
w	Velocity component	m/s
W	Weight function	
$\delta \mathbf{x}$	Position vector distance	m
$\mathbf{x}$	Position vector	m

Greek symbols

α	Volumetric phase fraction	
α_{mass}	Mass transfer coefficient	m/s
α_w	Gaussian distribution constant	
α_K	Kernel width coefficient	
β	Drag coefficient	
γ	Mass migration function	
Δ	Difference vector	
ε	Turbulent dissipation rate	m ² /s ³
ζ	Material properties	

η	Dynamic viscosity	Pa s
κ	Free surface curvature	1/m
λ	Thermal conductivity	W/(m K)
ν	Kinematic viscosity	m ² /s
ϱ	Density	kg/m ³
σ	Surface tension	N/m
$\sigma_k, \sigma_\varepsilon$	Coefficients in k- ε model	
τ	Strain rate tensor	1/s
ϕ, Φ	Arbitrary function	
φ	Relative humidity	%
Ψ	Species mass concentration or fraction	kg/kg

Indices

air	Air attribute
C	Value for control volume C
NC	Value for neighboring control volume NC
f	Center of face f
i, j	Counting index
corr	Corrected value
dyn	Dynamic attribute
hyd	Hydrostatic attribute
rg	Modified value
lam	Laminar fraction
radiation	Radiation fraction
turb	Turbulent fraction
eff	Effective value
vap	Water vapor attribute
water	Liquid water attribute
ϕ	Value for arbitrary function

Superscripts

n	Time step n
$\sim$	Discrete differential operator
$\wedge$	Preliminary value
sat	Saturation condition
∞	Function value in free stream or ambient condition

Dimensionless numbers

Nu	Nusselt number
Pr	Prandtl number
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number

Abbreviations

1D	One Dimensional
2D	Two Dimensional
3D	Three Dimensional
CD	Central Differencing
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy
DPM	Discrete Phase Model
FDM	Finite Difference Method
FPM	Finite Pointset Method
FVM	Finite Volume Method
GFDM	Generalized Finite Difference Method
MTC	Mass Transfer Coefficient
N-S	Navier-Stokes equation
PDE	Partial Differential Equation
PISO	Pressure Implicit with Splitting of Operators
RBF	Radial Basis Function
SIMPLE	Semi-Implicit Method for Pressure-Linked Equations
SPH	Smoothed Particle Hydrodynamics
TFA	Thin-Film Approximation
UD	Upwind Differencing
VoF	Volume of Fluid

1 Introduction

Accumulated water on solid surfaces, particularly metallic materials as shown in Figure 1.1, is one of the major sources of localized corrosion. Prolonged water stagnation in specific areas of the vehicle can initiate or accelerate the corrosion process. Such corrosion harms the durability of individual parts and, consequently, the overall lifespan of the vehicle itself. Therefore, to mitigate costs associated with the corrosion process, it is crucial to investigate in advance which parts are prone to becoming wet and for how long they remain in a wet state.



Figure 1.1: Wet surfaces of vehicle example

1.1 Motivation and Objective

Water evaporation below its boiling point is a common phenomenon that can be observed in everyday situations. However, accurately modeling and predicting the evaporation rate in numerical simulations is challenging due to the complex nature of the process.

It is a rather complex multi-physics heat- and mass-transferring process occurring at the phase interfacial free surface – water and air, depending on many different factors [SINGH & XU 1998]. Nonetheless, precisely estimating the evaporation rate and the total dry-out time under specific conditions are crucial for numerous industrial applications, including predicting localized corrosion in automotive components. Medium- and long-term water accumulation on the metallic surfaces of a vehicle can initiate and accelerate localized corrosion, which in the course of time harms the life span and durability of the entire vehicle [REVIE 2015, ROBERGE 2008].

Moreover, the automotive industry's shift from traditional internal combustion engines to battery-powered electric vehicles (EVs), which operate at lower temperatures, further

complicates the issue. As a result, any accumulated water on EV components may persist for longer periods after water exposure due to these lower operating temperatures [DAMKÖHLER 2011]."

Thus, developing a robust, flexible, and, ultimately, automated numerical method to resolve evaporation physics for automotive applications is required and has become more critical. Such a method would be essential for optimizing anti-corrosion strategies during the vehicle design phase, leading to significant reductions in both development time and costs. This will consequently save time and cost of development cycles.

1.2 Thesis Outline

The first part of this dissertation introduces previous works performed by many researchers that are related to this study (Chapter 2). In this chapter, various numerical methods that are used for Computational Fluid Dynamics (CFD), including the ones that are used for this study, are reviewed and compared.

Following that, previous researches that were carried out with the application of the CFD in the field of automotive industries are introduced, and what was lacking in these studies is discussed. Moreover, CFD methods developed for evaporation physics by previous researchers in various ranges of applications and their limitations are reviewed. Lastly, experimental investigations conducted to measure the evaporation rate in diverse fields are surveyed.

In Chapter 3, fundamental mathematical models used in the CFD, as well as the numerical models that are used for this specific research, are summarized. Then, thorough explanations regarding the development of the method to resolve evaporation physics in various possible approaches are described.

In the next part of this study, Chapter 4, the validation processes in terms of the calculated evaporation rate of the developed model with a relatively simple geometry are performed. For the validation, a series of experiments were designed and conducted. Here, the ambient conditions that highly influence the evaporation rate are varied, and the outcomes are compared with the simulated evaporation rates. Following that, the result is discussed, and the best method that fits the target application is determined.

In the following Chapter 5, the selected method is deployed to actual vehicle geometries. In order to validate, experiments are designed and performed to measure the total dry-out time of water accumulation at the corner of the sunroof channel of a vehicle.

Here, an artificial acceleration method to extend the time scale of the simulation into the real-world time scale is introduced and applied for the validation comparison. Further, the method is also used for a typical automotive application of simulating the effects on the dry-out time with different component design variations in different vehicle geometries.

Chapter 6 and 7 present examples of how the method can be extended to more complex vehicle geometries and how thermal boundary conditions can be accounted for. Finally, the findings of this dissertation are summarized, and the recommendations for further improvement directions are discussed.

1.3 General Remarks

- The FVM-based solver used in this investigation is called OpenFOAM developed by ESI Group.
- The version of the FVM-based solver OpenFOAM that is used for the investigation is v19.12.
- For the mesh generation, snappyHexMesh utility in OpenFOAM is used.
- The GFDM-based solver that is used in this study is called MESHFREE developed by Fraunhofer Institute for Industrial Mathematics ITWM and Fraunhofer Institute for Algorithms and Scientific Computing SCAI.
- Various versions, including beta versions for MESHFREE solver, are used for the research.

2 Literature Review

In this chapter, a literature review of the previous research in various fields that are related to the current study is conducted. The first part introduces various numerical methods used in CFD fields. Following that, the applications of CFD in the automotive sector are presented.

Next, the CFD research works carried out to resolve the evaporation phenomena in a diverse range of applications are surveyed. In the end, experimental studies to measure the evaporation rate in multiple fields are reviewed.

2.1 Numerical methods for CFD

In the field of Computational Fluid Dynamics (CFD), there exist two alternative mathematical descriptions to observe and analyze the motion of fluid – the Lagrangian and the Eulerian descriptions [ÇENGEL & CİMBALA 2013]. One of the most widely and traditionally used numerical methods in CFD is the Finite Volume Method (FVM), which describes the fluid motion in the Eulerian manner. This approach involves defining a finite volume known as a fluid domain, allowing fluid to enter and exit while the system monitors the fluid within this specified domain.

The FVM resolves the fluid motion characterized by field variables such as pressure and velocity, which vary with time and space, by sub-dividing the fluid domain into a number of smaller, non-overlapping sub-domains. These sub-divided control volumes are called discretized cells, and this pre-processing operation is called mesh generation or meshing process [ÇENGEL & CİMBALA 2013, VERSTEEG & MALALASEKERA 2007]. Thus, the methods that require the mesh generation process are called mesh-based methods.

Even though the meshing pre-processing is not trivial and often time-consuming, most numerical methods to date require mesh generation over the computational domain to resolve fluid mechanics since it is traditionally well-established in a wide range of applications, as well as its conservative inheritance.

Although these conventional mesh-based methods, such as FVM, thrive in various industrial and academic applications, many researchers have also developed meshless methods for many other specific purposes over the years. One of the earliest developed and extensively used meshless methods is called Smoothed Particle Hydrodynamics (SPH) [LIU & LIU. 2003].

SPH is a Lagrangian meshfree approach that discretizes the computational domain with mass-carrying particles. It was originally developed for astrophysical applications, where solid boundaries are not required. This implies one of the significant limitations of SPH. Due to its lack of inherent mechanisms for imposing various different boundary conditions, enforcing specific boundary conditions can be challenging or may require additional effort [GINGOLD & MONAGHAN 1977, SUCHDE 2018].

Radial Basis Functions (RBF) based methods are another popular meshless methods class. RBF-based methods deploy radial functions, whose values solely depend on the distance from a fixed point. The target function is estimated by combining a linear set of a single radial basis function at different translated points, and the function's derivatives are determined by the derivatives of these incorporated radial basis functions [SUCHDE 2018].

MAI-DUY & TRAN-CONG 2001 and SARLER 2005 have deployed the RBF method to resolve Navier–Stokes equations and fluid mechanics in their studies. A drawback of RBF-based methods is that the accuracy and stability of the method significantly depend on the selection of the basis functions and their shape parameters [MONGILLO 2011]. Numerous studies, including FASSHAUER & ZHANG 2007, HOSSEINI ET AL. 2014 and HOSSEINI ET AL. 2022, introduce various concepts to improve the accuracy and stability/convergence of the method for many engineering and scientific applications. However, they are usually application-specific and ad-hoc in nature, which may require extra and expensive stabilization techniques depending on the choices of the radial basis function [SUCHDE 2018].

The last meshless method introduced in this thesis is a mesh-free collocation approach referred to as the Generalized Finite Difference Method (GFDM), also known as the Finite Pointset Method (FPM). GFDM generalizes finite difference methods (FDM) to arbitrary point distributions by employing weighted least squares approximations. In this context, the required derivatives to determine the flow regime are given by linear combinations of the function values at neighboring points [MICHEL ET AL. 2021].

It offers a straightforward way to integrate a diverse variety of boundary conditions, which is a considerable advantage over SPH. Furthermore, the derivatives in GFDMs are taken as linear combinations of function values. These methods do not directly rely on the derivatives of kernel functions, in contrast to RBF-generated finite differences (RBF-FD) or SPH, where the desired function derivatives are contingent upon the chosen radial basis function or kernel function, respectively [SUCHDE 2018].

2.2 Applications of CFD in automotive water management

In the automotive sector, air-only single-phase CFD simulations, more specifically FVM-based simulations, have been traditionally used in the fields of aerodynamics and aeroacoustics investigations over many years. Apart from the above applications, the

role of numerical methods that can effectively simulate free surface flows to analyze water management processes for vehicles has gained significance recently. They allow the optimization of water protection and management functionalities such as water drainage systems. This could also potentially minimize the local corrosion effects of vehicle components.

Key applications of simulations in automotive water management encompass water wading and fording [MAKANA ET AL. 2016, VARSHNEY ET AL. 2021], evaluating the impact of rainwater [KARBON & LONGMAN 1998, DASARATHAN ET AL. 2016, DEMEL ET AL. 2019], and cleaning of sensors for automated driving [DEMEL ET AL. 2021]. For such scenarios, the Volume of Fluid (VoF) multi-phase method is the most widely used method to resolve the free surface at the phase interface – air and water – in FVM-based approaches [DEMEL ET AL. 2021, DIANAT ET AL. 2017].

While the VoF approach thrives in the FVM-based world, meshfree methods are also gaining ground since they are sometimes more suitable for these applications due to the ease of handling free surfaces and large domain deformations [JEFFERIES ET AL. 2015, WICKERT ET AL. 2020].

The majority of the research in vehicle water management applications to date has concentrated on studying the dynamic behavior of water flowing along intricate external vehicle surfaces, such as during rainfall or water wading. These researches merely investigate which components come into contact with external water sources without assessing the wetness duration, which is the ultimate purpose of the present work.

2.3 CFD methods for evaporation physics

Numerous researchers have developed CFD methods for addressing multi-phase mass transfer phenomena occurring across phase interfaces for many different applications. WICKERT & PROKOP 2021 provided a state-of-the-art overview of already developed water evaporation solvers using several commercial CFD codes. They validated the simulation outcomes by conducting a simple experiment under only one ambient atmospheric condition – 35°C and 32% relative humidity – without any forced convection of air.

Furthermore, they analyzed and compared the performance as well as physical assumptions made upon different CFD codes. Nevertheless, a thorough evaluation of the performance of each commercial software package, particularly concerning the presence of forced air convection, is lacking in this review.

VIDAL-LÓPEZ ET AL. 2012 utilized CFD simulation with Ansys Fluent to examine the mass transfer coefficients, or wind functions, within a U.S. Class A evaporation pan, a standardized measurement instrument accredited by the U.S. National Weather Service. It should be noted that evaporation pans are containers filled with water and exposed to the atmosphere. Then, the loss of water mass resulting from the evaporation

process is measured at regular intervals. The study involved comparing these results with empirically derived wind functions.

LI & HEISELBERG 2005 as well as GALLERO ET AL. 2020 employed CFD simulation software to study and estimate water evaporation aspects in swimming pool applications. LI & HEISELBERG 2005 evaluated various water evaporation models using Ansys Fluent to access the mass flow rate of water evaporation and air-side humidity distributions in a swimming facility. This study aimed to optimize the ventilation system for indoor swimming pools and validated the findings with an actual swimming pool facility.

GALLERO ET AL. 2020 also used Ansys Fluent and introduced an improvement of a formerly proposed evaporation model for swimming pools by BLÁZQUEZ ET AL. 2017. These modifications aimed to improve accuracy, particularly in situations where forced convection plays a dominant role. GALLERO ET AL. 2020, LI & HEISELBERG 2005, and VIDAL-LÓPEZ ET AL. 2012 all conducted air-only single-phase simulations by imposing boundary conditions for the water surface instead of defining an explicit air-water interface, opting for simplicity.

However, this approach ultimately fails to precisely compute the actual decrease in water volume caused by evaporation. In contrast, in this current study, the water source for evaporation is present so that the reduction of the actual water volume can be accurately calculated.

KUMAR ET AL. 2020, RAGAB & WANG 2012 as well as SAUFI ET AL. 2019 developed and investigated evaporation models specifically designed for liquid droplets, encompassing water or fuel. KUMAR ET AL. 2020 utilized the Discrete Phase Model (DPM) in Ansys Fluent to study the droplet evaporation behavior for applications such as spray cooling, scramjet combustion, and fuel injection.

SAUFI ET AL. 2019 developed a comprehensive computational solver in OpenFOAM, called DropletSMOKE++, designed to analyze the evaporation process of fuel droplets using the VoF method. There, the evaporation rate is directly evaluated by assessing the vapor concentration gradient at the phase interface.

RAGAB & WANG 2012 proposed an enhanced evaporation method to improve the accuracy of the resulting temperature during the evaporation calculation. This approach was compared with the built-in default droplet evaporation model integrated into Ansys Fluent.

YANG & KONG 2017 and WANG ET AL. 2020 investigated evaporation models for the liquid droplets using SPH. YANG & KONG 2017 proposed a general approach for modeling evaporating multiphase flows that are discretized using SPH particles. Here, the mass transfer rate from liquid to gas particle elements is computed according to the vapor concentration gradient as the current study. The 2D simulation results were then compared with findings in existing literature.

WANG ET AL. 2020 also introduced a 2D SPH framework of the liquid fuel droplet evaporation within the context of the combustion process. They adopted the Fourier

heat conduction equation and Fick's law of diffusion for the heat and mass transfer calculation. The single droplet simulation results are validated with the experiment.

The collective studies on evaporation phenomena (KUMAR ET AL. 2020, RAGAB & WANG 2012, SAUFI ET AL. 2019, WANG ET AL. 2020, YANG & KONG 2017) concentrate on the analysis of microscopic physical aspects of evaporation in individual single small-sized droplet within the range of μm to mm for applications such as spray cooling or fuel injection in combustion engines. In these applications, the intended scale of the evaporation source is considerably smaller, and the temperature conditions are notably higher compared to the intended application in the present study.

Furthermore, while some researchers such as SAUFI ET AL. 2019 and YANG & KONG 2017 computed the mass transfer rate by utilizing the vapor concentration gradient at the interface, their outcomes were not extensively validated on a larger scale, particularly in relation to diverse atmospheric ambient conditions.

LAAROUSSI ET AL. 2008 conducted numerical simulations in a vertical parallel-plate channel with evaporation occurring from thin liquid films on wet walls. The study's objective was to assess the impact of density variation and buoyancy forces arising from the evaporation of thin films from wet walls inside the channel, which is deployed in industrial heat exchanger applications. Instead of the conventional formulations based on the Boussinesq approximation, LAAROUSSI ET AL. 2008 employed a non-Boussinesq formulation in their simulations to ensure accurate prediction of flow structures.

SOSNOWSKI ET AL. 2013 extended the research by combining the thermal effects of both evaporation and condensation at the same time on the vertical parallel-plate channel. The effects of the thermal exchange between the wet air and the solid wall are implemented in OpenFOAM.

However, in both works ([LAAROUSSI ET AL. 2008] and [SOSNOWSKI ET AL. 2013]), it is assumed that the thickness of the water film on the solid is negligible. Thus, these studies focused only on the thermal effects of evaporation and condensation, which would impact the airflow characteristic inside the pipe and the thermal exchange rate between the solid wall without actual modeling of the water phase.

MEREDITH ET AL. 2011 included a water vaporization model (for both evaporation and boiling) in their Thin-Film Approximation (TFA) model, a greatly simplified multi-phase model to predict the transport of liquid over solid surfaces. This TFA model is implemented in a commercial open-source FVM code by taking into account the evaporation effects as a source term for inter-phase transport.

In this approach, the mass flux rate is calculated based on the user-defined mass transfer coefficient, which should be manually calculated based on the geometric configurations, and the evaporation model implemented was not thoroughly validated through the research. Moreover, The TFA model itself could become unstable if the water thickness grows beyond the range of mm scale, which could be the case for the applicational purpose of this study [LEE 2020].

2.4 Experimental evaporation process measurement

Historically, Dalton's set of experiments conducted in 1802 [DALTON 1802], measuring the evaporation rate, is regarded as one of the earliest reasonably accurate experiments in assessing the evaporation process [BAGHERI 2019]. Based on the measurements, Dalton formulated an equation to estimate evaporation [DALTON 1802], taking into account factors such as horizontal-directional wind speed, roughness of the surface, and thermally induced turbulence as

$$E_0 = C(e_s - e_a), \quad (2.1)$$

where E_0 is free surface evaporation, e_s is the saturation vapor pressure at the temperature of the water surface, e_a is the vapor pressure in the air and C is aerodynamic conductance.

As noted by various researchers, including SINGH & XU 1997, Dalton's formula is considered to be the fundamental principle underlying all derived mass-transfer methods or theories.

Several researchers, including FITZGERALD 1886, MEYER 1915, ROHWER 1931, HARBECK 1962, and KONSTANTINOV 1966, have sought to enhance the empirical accuracy of estimating the evaporation rate [SINGH & XU 1997b]. However, all these researches on the evaporation rate measurements are conducted in agricultural water reservoirs or lakes, whose surface areas are in the scale of acres (1 acre = 4046m²). This is way beyond the target scale of the current research, and due to various limitations of the formulae, they can be expected to only give an approximate magnitude of the evaporation [SUBRAMANYA 2008].

Another group of studies to evaluate the evaporation rate are performed with evaporation pans or evaporimeters. They are the most widely used method to directly measure the evaporation rate [STANHILL 2002]. While four types of evaporation pans (U.S. Class A evaporation Pan, ISI Standard evaporation Pan, Colorado Sunken Pan, and U.S. Geological Survey Floating Pan) are widely employed, several additional types of evaporation pans also exist [SUBRAMANYA 2008].

Numerous papers and articles discuss experiments conducted with evaporation pans, given its widespread use as the most common method. For example, MASONER ET AL. 2008 conducted an experiment to observe the difference in evaporation rate of two different evaporation pans – floating- and Class A evaporation pans – types deployed at a natural wetland. Considering the size of the evaporation pans (internal diameter of roughly 120cm and a depth of roughly 25cm), the scope of the studies is still way beyond the target scale of this current study.

CHU ET AL. 2010 conducted a set of wind tunnel experiments by deploying a Class A evaporation pan in an open-type wind tunnel, aiming to assess the evaporation rate under varying airflow rates (wind speed) and water depths.

HISATAKE ET AL. 1993 conducted a series of experiments to investigate how the evaporation rate of water in a small vessel is influenced by factors such as temperature, humidity, airflow rate, and vessel size. In their first experiment, the airflow was generated by a conventional fan, and it was blown parallel to the water surface.

Given the susceptibility to errors inherent in this experimental setup, HISATAKE ET AL. 1995 enhanced the accuracy in the subsequent experiment by using a wind-tunnel instead of a conventional fan. In contrast to prior experiments conducted by HISATAKE ET AL., HISATAKE ET AL. 1993, 1995, where one variable was fixed for each measurement series while the other two were varied (e.g., maintaining a fixed 40% relative humidity and measuring evaporation rates with varying air temperatures and flow rates), all three variables are adjusted and swept in the experiment done in the current investigation.

Moreover, the experimental work in the literature typically measures the water temperature at the air-water interface using a thermocouple. In contrast to this, the temperature of the water body is assessed in this study, which is then used as an initial condition in the simulations for more accurate validation results.

3 Background theories and methodologies

Parts of this section have been published in a similar way in:

Lee, J.; Bäder, D.; Rehfeldt, S.; Eisenträger, A.; Kuhnert, J.; Michel, I.; Suchde, P.; Klein, H.: *Modeling evaporation with a meshfree collocation approach*. Computational Particle Mechanics 10 (2023), pp. 1989–2007. DOI: 10.1007/s40571-023-00602-0.

Lee, J.; Bäder, D.; Rehfeldt, S.; Klein, H.: *Water Evaporation CFD Method with the Meshfree Volume-Volume-Coupling Approach for Wet Automotive Component Dry-Out Time Prediction*. International Journal of Automotive Engineering 15.1 (2024), pp. 58–65. DOI: 10.20485/jsaeijae.15.1_58.

Lee, J.; Bäder, D.; Rehfeldt, S.; Klein, H.: *VOF-based concentration-gradient-driven mass transfer model for water evaporation*. 10th OpenFOAM Conference. ESI Group. Nov. 2022.

In this thesis, new mass transfer models to simulate the below-boiling point evaporation of water implemented in a GFDM and the FVM are introduced. For a meshless GFDM approach, water-only single-phase and air-water multi-phase evaporation models are implemented since GFDM is able to capture the free surface of the water without the need to explicitly simulate the surrounding air phase, unlike the FVM. Two different coupling approaches are investigated for the multi-phase simulations – the surface-surface- and the volume-volume-coupling.

For the mesh-based FVM approach, the Volume of Fluid (VoF) multi-phase model is adopted to simulate both phases as well as the free surface. In this context, the mass transfer model is implemented at the phase interface.

In the single-phase simulations, the convective mass transfer theory is used in order to approximate the effect of the bulk air movement upon the mass transfer rate since the air phase is not resolved explicitly. For the multi-phase scenarios in both investigated methods (GFDM and FVM), it is assumed that the main driving force of the liquid mass transfer into vapor is diffusion due to the vapor concentration gradient in the air in the vicinity of the free surface of the water [CHEN ET AL. 2018]. Thus, semi-empirical evaporation submodels such as mass transfer coefficient (MTC) are not required as in convective mass transfer.

3.1 Brief background physical theories

In this section, the background physical theories that are related to this current study are briefly introduced.

3.1.1 Theories of evaporation

A substance that maintains a fixed chemical composition or a homogeneous mixture throughout is referred to as a pure substance. This pure substance can exist in three primary phases – solid, liquid, and gas [ÇENGEL ET AL. 2016]. As water (H_2O) is considered a pure substance, it can exist in any of these forms – ice, liquid water, or vapor.

The transition of liquid water between phases under constant pressure, particularly at 1 atm, is illustrated in Figure 3.1 as it undergoes heating from an external heat source.

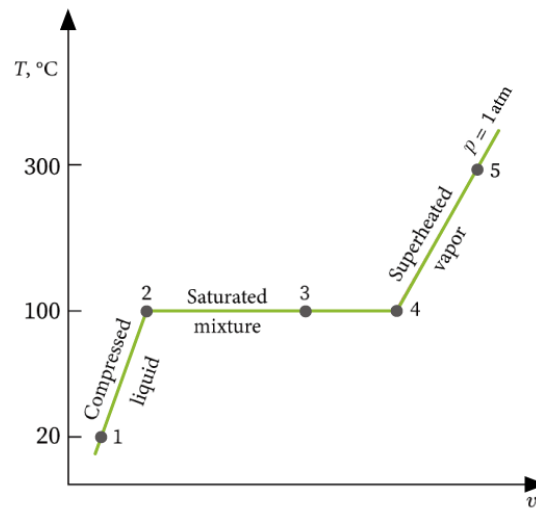


Figure 3.1: Temperature vs. specific volume diagram at 1 atm. Adapted from [ÇENGEL ET AL. 2016].

The process by which a substance changes its phase from liquid to gaseous form is called the vaporization process. This vaporization process can be categorized into two familiar terms:

- Boiling
- Evaporation

Even though both terms are used for the liquid-to-vapor phase change process, significant differences exist. Boiling occurs at solid-liquid interfaces when the solid surface temperature is higher than the saturation temperature T_{sat} of the liquid. On the other hand, evaporation takes place at the free surface when the vapor pressure is less

than the saturation pressure of the liquid, even if the temperature is lower than the boiling point [ÇENGEL 2002].

A substantial amount of energy, specifically in the form of heat, is required to achieve the mass transfer between liquid-to-vapor for a pure substance. The energy absorbed or released during the phase-change process is called *latent heat*. Specifically, the latent heat absorbed during the vaporization process of water is referred to as the *latent heat of vaporization* [ÇENGEL & GHAJAR 2014, ÇENGEL 2002, ÇENGEL ET AL. 2016]. The latent heat of vaporization of water is $2257.1 \frac{\text{kJ}}{\text{kg}}$ at 1 atm pressure [ÇENGEL ET AL. 2016]

This evaporation process at the free surface takes place even below the boiling temperature since there always exist some surface molecules that have sufficient energy to break the liquid bound by the Maxwell-Boltzmann distribution [GERASIMOV & YURIN 2018]. Consequently, molecules in the liquid are separated from their neighboring molecules and transition into the vapor state. This non-equilibrium process will continue until the vapor partial pressure reaches the saturation pressure at the given temperature, i.e., 100% relative humidity. Thus, the local evaporation rate at the free surface is highly affected by the surrounding relative humidity.

However, the complexity of the evaporation process increases significantly in practical scenarios. This process is greatly influenced by meteorological factors such as temperature, wind speed, atmospheric pressure, solar radiation, the chemical and physical quality of the water (including factors such as salinity, turbidity, and the presence of impurities), and the configuration of the evaporating surface [MORTON 1968]. Thus, in practical engineering problems, a sophisticated numerical approach to resolve this evaporation physics rather than a theoretical approach is required.

3.1.2 Theories of localized corrosion

Corrosion is commonly referred to as rusting and tarnishing on solid metallic surfaces. In reality, corrosion damages can lead to failures through processes such as cracking or the loss of strength and ductility [REVIE 2015]. Therefore, ensuring adequate corrosion protection for vehicles is crucial as it safeguards not only the functionality of components but also the safety of drivers and passengers.

The corrosion process can be identified by its characteristics. A commonly employed method for identifying the types of corrosion involves visual examination and subsequent categorization into the following [ROBERGE 2008]:

- Uniform/general corrosion
- Localized corrosion
- Galvanic corrosion

Uniform corrosion, also known as general corrosion, refers to the consistent and uniform loss of metal from the surface. In contrast, localized corrosion represents any form of corrosion that occurs at specific sites on the metal surface. Galvanic corrosion occurs

through the electrical contact between dissimilar conductors in an electrolyte [ROBERGE 2008, SCHWEITZER 2004].

Given the relevance of localized corrosion to this study, additional discussion on localized corrosion will be presented. Localized corrosion can be categorized into the following types – pitting and crevice corrosion.

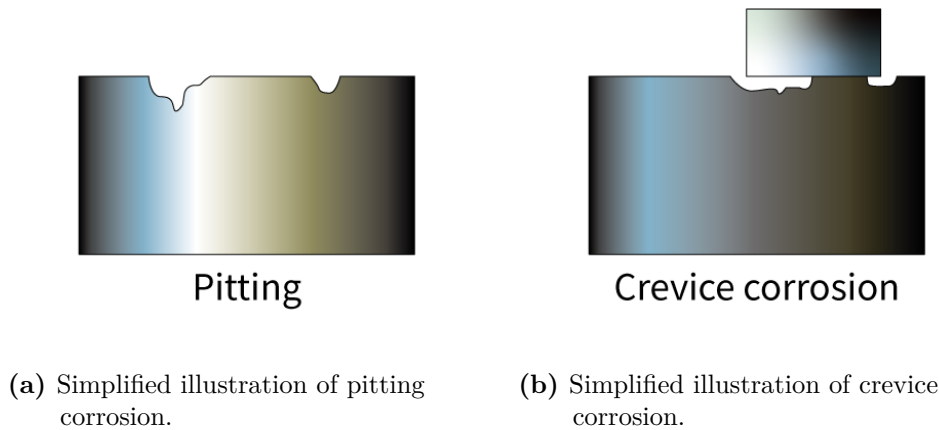


Figure 3.2: Localized corrosion illustrations. Adapted from [ROBERGE 2008].

Pitting represents an extremely localized form of corrosion and stands out as one of the most destructive corrosion types. Corrosion pits are formed as small cavities or holes on the metal surface, as depicted in the illustration in Figure 3.2a. This pitting corrosion may be initiated by stagnant or slowly flowing liquid on the metal surface [ROBERGE 2008].

Crevice corrosion is an additional form of localized corrosion, often taking place within or near narrow gaps referred to as crevices. These crevices can be between metal-to-metal or metal-to-nonmetal contacts, as depicted with a simplified illustration in Figure 3.2b. The crevice corrosion can be triggered by the accumulation of a small amount of liquid that becomes stagnant in crevices, such as beneath bolt gaskets or around rivet heads.

Once these local corrosion types are initiated, the corrosion area grows rapidly into various forms, and this process can be accelerated by the existence of water on the damaged areas [POPOV 2015, SCHWEITZER 2004].

The following list highlights common areas on a vehicle that are prone to such types of localized corrosion[BAGHERI 2019]:

- Brake lines
- Struts and shocks
- Wheel arches
- Roof and sunroof drainage channel
- Fenders
- Door locks and handles
- Window pillars

The localized corrosion types introduced in this section can be mitigated by effective vehicle component design, aiming to minimize water accumulation as well as to create favorable evaporation conditions. This, in turn, leads to extended lifespans for vehicle parts and results in cost savings in manufacturing.

3.2 Computational Fluid Dynamics

In general, it is obvious that numerical simulation tools and techniques for the progress of technology and science have become crucial to the development of a wide range of today's technologies. Computational Fluid Dynamics (CFD) is one of these simulation tools. Even though it was initially developed for the aeronautics and aerospace industry, it has evolved into a crucial tool in various other design-intensive industrial sectors, including automotive, power generation, chemical, nuclear, and marine industries, to name a few [MOUKALLED ET AL. 2016].

CFD is a numerical approach to solve the equations that describe the fluid motion, which do not have analytic solutions to date. There are various kinds of discretization methods available, depending on the problems. Traditionally, the finite volume discretization method is widely used. However, other discretization methods, such as SPH or GFDM, are also gaining their positions in this field.

3.3 Fundamental governing equations

The fundamental set of governing equations that describes the fluid dynamics is called *Navier-Stokes equations* (N-S). Historically, the *Navier-Stokes equations* only refer to the momentum equations for a viscous fluid where viscous stress exists. However, in the context of modern CFD, this terminology indicates the entire system of equations, including continuity and energy, as well as momentum equations in general [ANDERSON 1995].

Each equation – continuity, momentum, and energy – depicts fundamental physical principles as follows [ANDERSON 2010] :

- Mass is conserved.
- Momentum is conserved. ($\mathbf{F} = m\mathbf{a}$ – Newton's 2nd Law)
- Energy is conserved.

The governing equations for fluid dynamics, known as N-S equations, do not have a universal analytic solution for pressure, velocity components, and energy yet to date [ANDERSON 2010, ANDERSON 1995]. Consequently, a common method to tackle these equations involves numerical solutions that approximate the solution via discretization in both time and space. Full detailed explanations and derivation process of N-S equations can be found in [VERSTEEG & MALALASEKERA 2007, ANDERSON 1995, ANDERSON 2010].

The fundamental governing equations for modeling both the water and air phases are the standard conservation equations for mass, momentum, and energy. The equations are given as follows, noting that the equations are in Lagrangian time derivative form or the material time derivative form [JEFFERIES ET AL. 2015]:

$$\begin{aligned}\frac{d}{dt}\varrho + \varrho \nabla^T \mathbf{v} &= 0, \\ \frac{d}{dt}(\varrho \mathbf{v}) + (\varrho \mathbf{v}) \nabla^T \mathbf{v} &= (\nabla^T \mathbf{S})^T - \nabla p + \varrho \mathbf{g}, \\ \frac{d}{dt}(\varrho E) + (\varrho E) \nabla^T \mathbf{v} &= \nabla^T (\mathbf{S} \mathbf{v}) - \nabla^T (p \mathbf{v}) + \varrho \mathbf{g}^T \mathbf{v} + \nabla^T (\lambda \nabla T),\end{aligned}\tag{3.1}$$

where ϱ is the density, p is the pressure, $\mathbf{v}$ is the velocity vector, $\mathbf{S}$ is the stress tensor, $\mathbf{g}$ is the gravitational body force, E is the specific total energy, or $E = c_v T + \frac{1}{2}(\mathbf{v}^T \mathbf{v})$, c_v is the heat capacity. λ is the thermal conductivity, T is the temperature, ∇ is the gradient, and ∇^T is the divergence.

For the Eulerian time derivative form, commonly denoted by $\frac{\partial}{\partial t}$, the material derivative for any general functional value ϕ can be substituted with the following correlation: [VERSTEEG & MALALASEKERA 2007, JEFFERIES ET AL. 2015]

$$\frac{d\phi}{dt} = \frac{\partial \phi}{\partial t} + \mathbf{v}^T \nabla \phi = \frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi.\tag{3.2}$$

From the above general physical model, the stress tensor $\mathbf{S}$ can be splitted into solid and viscous parts in order to derive a useful numerical scheme as [JEFFERIES ET AL. 2015]

$$\mathbf{S} = \mathbf{S}_{\text{solid}} + \mathbf{S}_{\text{visc}}.\tag{3.3}$$

Since the solid part is not under consideration for the current specific application, only the viscous stresses are defined as

$$\mathbf{S}_{\text{visc}} = \eta \boldsymbol{\tau},\tag{3.4}$$

where η is the dynamic viscosity and $\boldsymbol{\tau}$ is the strain rate tensor, accounting for the local deformation rate of the fluid given by [JEFFERIES ET AL. 2015]

$$\boldsymbol{\tau} = \frac{1}{2} \left[\nabla \mathbf{v}^T + (\nabla \mathbf{v}^T)^T \right] - \frac{1}{3} (\nabla^T \mathbf{v}) \mathbf{I},\tag{3.5}$$

where $\mathbf{I}$ is the identity tensor.

For incompressible flows, the mass conservation equation can be written as

$$\nabla^T \mathbf{v} = 0.\tag{3.6}$$

3.4 Extension of governing equations

Apart from the fundamental N-S governing equations, a few more equations should be added to the system in order to correctly simulate the scenario that is investigated in the current study. These are the equations to take into account the turbulent effects and the species transport within a phase, specifically vapor in air.

3.4.1 Turbulence equations

The standard $k - \varepsilon$ model is deployed to incorporate turbulent effects [LAUNDER & SPALDING 1974] in the fluid dynamics. For that, equations for two more variables (turbulent kinetic energy k and turbulent dissipation rate ε) are added as [MICHEL ET AL. 2021],

$$\begin{aligned} \frac{dk}{dt} &= \frac{1}{\varrho} \nabla^T \left(\left(\eta + \frac{\eta_{\text{turb}}}{\sigma_k} \right) \nabla k \right) - \varepsilon + \frac{1}{\varrho} (P_{\text{pr}} + P_{\text{b}}), \\ \frac{d\varepsilon}{dt} &= \frac{1}{\varrho} \nabla^T \left(\left(\eta + \frac{\eta_{\text{turb}}}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) - C_{2\varepsilon} \frac{\varepsilon^2}{k} + \frac{1}{\varrho} C_{1\varepsilon} \frac{\varepsilon}{k} (P_{\text{pr}} + C_{3\varepsilon} P_{\text{b}}), \end{aligned} \quad (3.7)$$

where where

$$\begin{aligned} \eta_{\text{turb}} &= \varrho C_\eta \frac{k^2}{\varepsilon}, \\ P_{\text{pr}} &= \eta_{\text{turb}} \left\| \nabla \mathbf{v}^T \right\|_M^2, \\ P_{\text{b}} &= -\frac{1}{\varrho} \frac{\eta_{\text{turb}}}{Pr_{\text{turb}}} \frac{\partial \varrho}{\partial T} (\mathbf{g} \nabla T). \end{aligned} \quad (3.8)$$

Here, η is the laminar viscosity, and η_{turb} is the turbulent viscosity. The turbulent production rate is denoted as P_{pr} with von Mises matrix norm $\|\cdot\|_M$. P_{b} is the turbulent buoyancy, and Pr_{turb} is turbulent Prandtl number. The coefficient values are as following – $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $C_{3\varepsilon} = -0.33$, $C_\eta = 0.09$, noting that the fluctuating dilatation and source terms are omitted [LAUNDER & SPALDING 1974, MICHEL ET AL. 2021],

With the application of the turbulence model, the original stress tensor equation used for the N-S equation (3.4) is then extended as

$$\mathbf{S}_{\text{visc}} = (\eta + \eta_{\text{turb}}) \boldsymbol{\tau}. \quad (3.9)$$

3.4.2 Species transport equation

In order to simulate the species transport within a phase, the basic system of equations should be extended by convection-diffusion equations for the necessary species. For

the i -th ($i = 1, 2, \dots, N$) species concentration within a phase, the transport equation is given by

$$\frac{d\Psi_i}{dt} + \Psi_i \nabla^T \mathbf{v} = \nabla^T (D_{i,\text{eff}} \nabla \Psi_i) + S_i, \quad (3.10)$$

where Ψ_i is the concentration of i -th species and $D_{i,\text{eff}} = D_{i,\text{lam}} + D_{i,\text{turb}}$ represents the effective diffusivity of the i -th species within the phase, incorporating with the effects of turbulent diffusivity. S_i is the source term of the i -th species such as mass source generated from the free surface of water into the air by evaporation.

In this specific context, only one species concentration is present, i.e. vapor concentration within the air phase. Thus, only one equation is required.

3.5 Fluid modeling: single- and multi-phase

The term single-phase flow in fluid dynamics refers to fluid flow with only one phase or component whose physical properties are identical, for instance, gaseous air or liquid water. At the boundaries of the flow, physical properties are controlled by the user-specified boundary conditions. The term multi-phase flow, on the other hand, is used for any fluid flow consisting of more than one phase that has the phase separation at a scale well above the molecular level – e.g., gas-liquid or solid-gas [BRENNEN 2005].

Furthermore, apart from the boundary conditions, these phases interact with each other at the interface in some sense, for example, for the calculation of momentum, mass, and thermal transfer to resolve the underlying physics. In this thesis, both approaches are considered for the investigation. For the single-phase flow (in the GFDM approach), only the water phase is considered, and evaporation physics are approximated by the imposed boundary conditions at the given atmospheric conditions, whereas, for the multi-phase flow (in both GFDM and FVM approaches), the evaporation phenomenon is resolved by the exact interactions between the phases. Detailed explanations of different phase coupling models are elaborated in the following sections: Section 3.6.3, 3.6.3, and 3.7.2.

3.6 Modeling and Implementations in GFDM

The meshless computational framework used for this study is the CFD simulation software suite named MESHFREE developed by Fraunhofer ITWM and SCAI [MESHFREE TEAM 2023], which is based on a Generalized Finite Difference Method (GFDM) and has also been referred to as the Finite Pointset Method (FPM) in the past [JEFFERIES ET AL. 2015]. In this framework, a new model to simulate the water evaporation physics is implemented.

3.6.1 Generalized Finite Difference Method

The Generalized Finite Difference Method is a meshless numerical approach to resolve partial differential equations (PDE). This method employs a collocation of numerical points, with each point containing essential numerical data. Solving PDEs or fluid dynamics requires the computation of approximations for derivatives facilitated by a dedicated least-squares algorithm. The incorporation of the least squares concept transforms the entire method into a generalized finite difference approach. Detailed descriptions of each step are in the following section.

Domain discretization

The computational domain is discretized into a scattered set of $NP = NP(t)$ number of points, generally referred to as a point cloud, without any underlying interconnecting mesh topology. Scattered points are used to discretize the entire computational domain, including not just the interior but also domain and interface boundaries.

The density of the point cloud is determined by a sufficiently smooth function $h = h(\mathbf{x}, t)$, commonly referred to as the interaction radius or smoothing length. Hence, h prescribes the resolution of the point cloud and is also used to search neighborhoods for each point. For a point i , located in $\mathbf{x}_i$ within the point cloud, all approximations are performed solely with nearby points located within a distance h from it. This collection of nearby points is referred to as the neighborhood or denoted as $N_i = \{\mathbf{x}_l : \|\mathbf{x}_l - \mathbf{x}_i\|_2 \leq h(\mathbf{x}_i)\}$ [KUHNERT ET AL. 2017].

In order to guarantee an adequate quality of the point cloud, measures are taken to ensure that the distance between any two points is not less than $r_{\min} \cdot h$ and that every sphere with a radius of $r_{\max} \cdot h$ in the domain contains at least one point. Thus, the distance between each point and its nearest neighbor falls within the range of $r_{\min} \cdot h$ to $r_{\max} \cdot h$. Usually, $r_{\min} = 0.2$ and $r_{\max} = 0.4$ are used, which results in roughly 40 – 50 neighboring points for each interior point and lesser at and nearby the boundaries [DRUMM ET AL. 2008, MICHEL ET AL. 2021].

The initial quality of the point cloud, guaranteed by the aforementioned criteria, must be maintained throughout the simulation. These inter-point criteria, however, can be violated due to the Lagrangian movement of each point with the fluid velocity. This occurs through the accumulation or scattering of points, which could harm the quality of the numerical outcomes. To avoid this, points are inserted into regions with insufficient points and merged in areas of accumulation. This distortion correction method is entirely localized and significantly computationally cheaper than the remeshing process employed in mesh-based methods [DRUMM ET AL. 2008, KUHNERT 2014].

In multi-phase simulations, each phase is discretized by a separate point cloud, and the interactions between the phases are calculated at the phase interface explicitly. Examples of point cloud discretizations are shown in Figures 3.3 and 3.4 for the single-phase and multi-phase (with the surface-surface-coupling) cases, respectively. All point clouds

used in this thesis are generated using a meshfree advancing front procedure [LÖHNER & OÑATE 2004, SUCHDE ET AL. 2022].

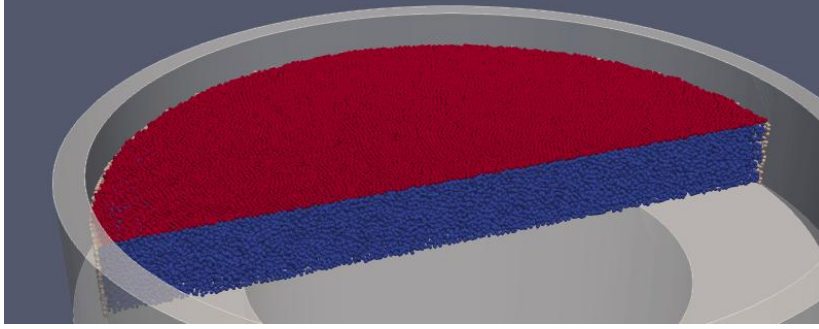


Figure 3.3: Domain discretization with two point clouds for the single-phase simulations. The color indicates different types of points: interior points (blue), free surface points (red), and wall boundary points (white). Only a clip of the full point cloud is shown. Adopted from [LEE ET AL. 2023a].

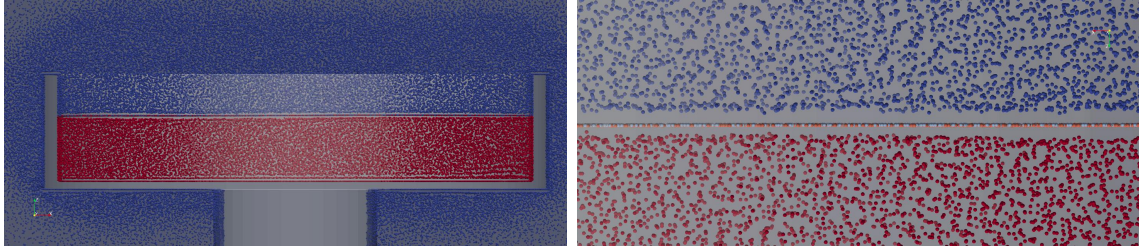


Figure 3.4: Domain discretization with a point cloud for the multi-phase simulations. The color indicates the different phases: air phase (blue) and water phase (red). Points of both phases are present at the interface, marked with lighter shades of blue and red, respectively. This figure shows the surface-surface-coupling case as an example. Adopted from [LEE ET AL. 2023a].

Construction of differential operators

The computation of numerical derivatives is conducted through a GFDM, employing a collocation approach that discretizes the governing equations in their strong formulation [FAN ET AL. 2018, GAVETE ET AL. 2017, LISZKA & ORKISZ 1980]. As the name suggests, the GFDM extends the classical finite differences to scattered point clouds without regular placement. At a numerical point i , positioned at $\mathbf{x}_i$, all derivatives are computed as weighted sums of function values at neighboring points. Thus, the required derivatives of an arbitrary function ϕ are approximated as

$$\partial^* \phi(\mathbf{x}_i) \approx \tilde{\partial}_i^* \phi = \sum_{j \in N_i} c_{ij}^* \phi_j = (\mathbf{c}_i^*)^T \boldsymbol{\phi}. \quad (3.11)$$

where ∂^* is the continuous derivative being approximated such as

$$\begin{aligned} \mathbf{c}_i^0 &= \text{the numerical operator for function approximation} \\ \mathbf{c}_i^x &= \text{the numerical operator for } x\text{-derivative} \\ \mathbf{c}_i^y &= \text{the numerical operator for } y\text{-derivative} \\ \mathbf{c}_i^z &= \text{the numerical operator for } z\text{-derivative} \\ \mathbf{c}_i^\Delta &= \text{the numerical operator for the Laplacian.} \end{aligned} \quad (3.12)$$

The numerical derivative at point i is represented by $\tilde{\partial}_i^*$ and ϕ_i is the function value at point i , or $\phi_i = \phi(\mathbf{x}_i)$.

The coefficients $\mathbf{c}_{ij}^*$ represent numerical differential operators, and they remain independent of the function being differentiated. The Taylor series expansion around point i at each neighboring point $j \in N_i$ is denoted as

$$e_{ij} + \phi(\mathbf{x}_j) = \phi(\mathbf{x}_i) + \nabla\phi \cdot (\mathbf{x}_j - \mathbf{x}_i) + \frac{1}{2} \nabla^2\phi(\mathbf{x}_j - \mathbf{x}_i)^T(\mathbf{x}_j - \mathbf{x}_i) \quad (3.13)$$

where e_{ij} refers to the errors in the Taylor series. The unknown coefficients $\nabla\phi$ and $\nabla^2\phi$ are calculated using a weighted least squares method by minimizing

$$\min J_i = \sum_{j \in N_i} W_{ij} e_{ij}^2, \quad (3.14)$$

where W_{ij} is a weight function employed to ensure that points close to the considered point (i) exert a greater impact than those located farther away. Thus, a Gaussian distribution is taken as

$$W_{ij} = \begin{cases} \exp\left(-\alpha_w \frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{h_i^2 + h_j^2}\right), & \text{if } \mathbf{x}_j \in N_i \\ 0, & \text{elsewhere} \end{cases} \quad (3.15)$$

where $\alpha_w \in [2, 8]$ [SUCHDE 2018]. It should be noted that the weight function is only defined on the local support N_i that consists of $n(i)$ points.

Equation (3.13) is reformulated as the following system, which is solved at each point $i \in (1, \dots, NP)$

$$\underbrace{\begin{pmatrix} e_{i1} \\ \vdots \\ e_{iNP} \end{pmatrix}}_{\mathbf{E}_i} = \underbrace{\begin{pmatrix} \delta x_{i1} & \frac{1}{2}\delta x_{i1}^2 \\ \vdots & \vdots \\ \delta x_{iNP} & \frac{1}{2}\delta x_{iNP}^2 \end{pmatrix}}_{\mathbf{M}_i} \underbrace{\begin{pmatrix} (\phi_x)_i \\ (\phi_{xx})_i \end{pmatrix}}_{\mathbf{a}_i} - \underbrace{\begin{pmatrix} \phi_1 - \phi_i \\ \vdots \\ \phi_{NP} - \phi_i \end{pmatrix}}_{\mathbf{b}_i}, \quad (3.16)$$

where $\delta x_{ij} = x_j - x_i$, and ϕ_x, ϕ_{xx} refer to the first and second x -derivative of the function. Note that this system only represents 1D cases for simplification. Equation (3.16) is

written in matrix-vector form as $\mathbf{E}_i = \mathbf{M}_i \mathbf{a}_i - \mathbf{b}_i$. Hence, the minimization equation (Equation (3.14)) is rewritten as

$$\min J_i = \mathbf{E}_i^T \mathbf{W}_i \mathbf{E}_i = (\mathbf{M}_i \mathbf{a}_i - \mathbf{b}_i)^T \mathbf{W}_i (\mathbf{M}_i \mathbf{a}_i - \mathbf{b}_i), \quad (3.17)$$

where $\mathbf{W}_i$ is a diagonal matrix, whose diagonal entries are $w_{i1}, \dots, w_{iNP}$, noted as

$$\mathbf{W}_i = \begin{pmatrix} w_{i1} & 0 & \dots & 0 \\ 0 & w_{i2} & & \\ \vdots & & \ddots & \\ 0 & & & w_{iNP} \end{pmatrix}, \quad (3.18)$$

where the diagonal entries are $(w_{i1}, \dots, w_{iNP})$ the discrete weights and zeros otherwise.

Formal minimization achieved by $\frac{\partial J_i}{\partial \mathbf{a}_i} = 0$ results in

$$\mathbf{a}_i = \left[(\mathbf{M}_i^T \mathbf{W}_i \mathbf{M}_i)^{-1} \mathbf{M}_i^T \mathbf{W}_i \right] \mathbf{b}_i, \quad (3.19)$$

which yields the differential operator stencils as [SUCHDE ET AL. 2018]

$$\begin{aligned} (\phi_x)_i &= \sum_{j \in N_i} c_{ij}^x (\phi_j - \phi_i), \\ (\phi_{xx})_i &= \sum_{j \in N_i} c_{ij}^{xx} (\phi_j - \phi_i), \end{aligned} \quad (3.20)$$

where,

$$\begin{pmatrix} \dots & c_{ij}^x & \dots \\ \dots & c_{ij}^{xx} & \dots \end{pmatrix} = \left[(\mathbf{M}_i^T \mathbf{W}_i \mathbf{M}_i)^{-1} \mathbf{M}_i^T \mathbf{W}_i \right]. \quad (3.21)$$

Alternatively, Equation (3.16) can be written as

$$\underbrace{\begin{pmatrix} e_{i1} \\ \vdots \\ e_{iNP} \end{pmatrix}}_{\mathbf{E}_i} = \underbrace{\begin{pmatrix} 1 & \delta x_{i1} & \frac{1}{2} \delta x_{i1}^2 \\ \vdots & \vdots & \vdots \\ 1 & \delta x_{iNP} & \frac{1}{2} \delta x_{iNP}^2 \end{pmatrix}}_{\mathbf{M}_i} \underbrace{\begin{pmatrix} (\phi_0)_i \\ (\phi_x)_i \\ (\phi_{xx})_i \end{pmatrix}}_{\mathbf{a}_i} - \underbrace{\begin{pmatrix} \phi_1 \\ \vdots \\ \phi_{NP} \end{pmatrix}}_{\mathbf{b}_i}, \quad (3.22)$$

where the derivative stencils are derived as

$$\begin{aligned} (\phi_0)_i &= \sum_{j \in N_i} c_{ij}^0 \phi_j, \\ (\phi_x)_i &= \sum_{j \in N_i} c_{ij}^x \phi_j, \\ (\phi_{xx})_i &= \sum_{j \in N_i} c_{ij}^{xx} \phi_j. \end{aligned} \quad (3.23)$$

These stencil coefficients are then used to obtain the spatial discretization of the PDE that needs to be solved. For example, if the following PDE is considered

$$a\phi + b\phi_x + c\phi_{xx} = d, \quad (3.24)$$

the derivative approximations (Equation (3.20)) are substituted with the terms in the PDE as

$$a\phi_i + b \sum_{j \in N_i} c_{ij}^x (\phi_j - \phi_i) + c \sum_{j \in N_i} c_{ij}^{xx} (\phi_j - \phi_i) = d, \quad i = 1, \dots, NP. \quad (3.25)$$

This eventually forms a large sparse implicit matrix system, which can be solved with an iterative method. More details on the derivative computation procedure can be found in [SUCHDE 2018] and [KRAUS ET AL. 2022].

Time integration

The continuous spatial derivatives in the Lagrangian formulation of the governing equations, illustrated in Equation (3.1), are substituted with their numerical counterparts approximated through the least squares method for the time integration. In this context, the superscript n denotes the current time step, and $n+1$ stands for the next time step. The time step size is $\Delta t = t^{n+1} - t^n$.

- Step 1. Point cloud movement

The time-integration procedure starts with a discretization of the Lagrangian motion by moving each point with the corresponding velocity vector [SUCHDE & KUHNERT 2018]. For each point ($i = 1, \dots, NP$) movement, a second-order method is deployed as

$$\mathbf{x}_i^{n+1} = \mathbf{x}_i^n + \mathbf{v}_i^n \Delta t + \frac{1}{2} \frac{\mathbf{v}_i^n - \mathbf{v}_i^{n-1}}{\Delta t} (\Delta t)^2. \quad (3.26)$$

Note that the change in velocity between two time steps is taken into account solely for the purpose of point movement and not for the new velocity $\mathbf{v}_i^{n+1}$ computation, which is resolved by solving the PDEs. An additional movement of the free surface points according to the retraction velocity caused by evaporation, which is explained in Section 3.6.1, is imposed as an extra step after all point movement is calculated.

- Step 2. Physical properties update

The physical properties, such as density ϱ , diffusivity D_{eff} , and the heat capacity c_v , are updated in the second step. The physical properties of the water phase are assumed to be constant, while the properties of the air side can be denoted as

$$\begin{aligned} \varrho^{n+1} &= \Psi_{\text{vap}}^{n+1} \varrho_{\text{vap}} + (1 - \Psi_{\text{vap}}^{n+1}) \varrho_{\text{air}}, \\ c_v^{n+1} &= \Psi_{\text{vap}}^{n+1} c_{v,\text{vap}} + (1 - \Psi_{\text{vap}}^{n+1}) c_{v,\text{air}}. \end{aligned} \quad (3.27)$$

Other physical properties such as laminar dynamic viscosity η_{lam} are assumed to remain constant. The effective viscosity is also calculated in this step. More details regarding the diffusivity of vapor in air D_{eff} are provided in the following section (Section 3.6.3).

- Step 3. Hydrostatic pressure

The next step is to split the pressure into two different components such that

$$p = p_{\text{hyd}} + p_{\text{dyn}}, \quad (3.28)$$

where p_{hyd} denotes the hydrostatic pressure (body forces) and p_{dyn} is the dynamic pressure (movement of the fluid).

The hydrostatic pressure is calculated

$$\tilde{\nabla}^T \left(\frac{1}{\varrho^{n+1}} \tilde{\nabla} p_{\text{hyd}}^{n+1} \right) = \tilde{\nabla}^T \mathbf{g}. \quad (3.29)$$

This updated hydrostatic pressure is used for the predicted pressure $\hat{p}$ for the new velocity calculation as [MICHEL ET AL. 2021]

$$\hat{p} = p_{\text{hyd}}^{n+1} + p_{\text{dyn}}^n. \quad (3.30)$$

- Step 4. Temperature update

A semi-implicit time integration is then conducted to calculate the updated temperature T^{n+1} as

$$\begin{aligned} (\mathbf{I}_T + \mathbf{D}_T) T^{n+1} &= (\varrho^n c_v^n) T^n + f_T, \\ \text{where} \\ \mathbf{I}_T &= \varrho^n c_v^n \mathbf{I}, \\ \mathbf{D}_T &= -\Delta t \tilde{\nabla}^T (\lambda \tilde{\nabla}^T), \\ f_T &= \Delta t \left(\tilde{\nabla}^T (\mathbf{S}^n \cdot \mathbf{v}^n) - (\tilde{\nabla}^T \mathbf{S}^n) \cdot \mathbf{v}^n - p^n \tilde{\nabla}^T \mathbf{v}^n \right), \end{aligned} \quad (3.31)$$

where $\mathbf{I}$ is the identity matrix, $\sim$ denotes the discrete differential operators, and point index i is omitted for simplification. Also note that the energy conservation equation is rewritten in the temperature form with $E = c_v T + \frac{1}{2} (\mathbf{v}^T \mathbf{v})$. Equation (3.26) yields a sparse linear system of equations with unknowns T^{n+1} for each point in the point cloud. All resultant implicit linear systems are solved with a BiCGSTAB solver without the use of any pre-conditioner [VAN DER VORST 1992].

- Step 5. Velocity-pressure coupling

First, the numerical formulation of the time derivative of velocity in momentum equations using the aforementioned predicted pressure $\hat{p}$ is given by

$$\begin{aligned} \frac{\hat{\mathbf{v}}^{n+1} - \mathbf{v}^n}{\Delta t} &= \frac{1}{\varrho^{n+1}} \left(\tilde{\nabla}^T \mathbf{S}_{\text{visc}}^{n+1} \right)^T - \frac{1}{\varrho^{n+1}} \tilde{\nabla} \hat{p} + \mathbf{g}, \\ \mathbf{S}_{\text{visc}}^{n+1} &= \eta \boldsymbol{\tau}^{n+1}, \end{aligned} \quad (3.32)$$

where $\hat{\mathbf{v}}^{n+1}$ is preliminary velocity, noting that it is a first-order time approximation notation for simplicity. The expression is rearranged as

$$\begin{aligned} \left(\mathbf{I} - \frac{\Delta t}{\varrho^{n+1}} \tilde{\Theta}^{n+1} \right) \hat{\mathbf{v}}^{n+1} &= \mathbf{v}^n - \frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} \hat{p} + \Delta t \mathbf{g}, \quad \text{where} \\ \left(\tilde{\Theta}^{n+1} \right)^T &= \tilde{\nabla}^T \left(\eta \tilde{\nabla} \right) \left(\hat{\mathbf{v}}^{n+1} \right)^T + \left(\tilde{\nabla} \eta \right)^T \left(\tilde{\nabla} \left(\hat{\mathbf{v}}^{n+1} \right)^T \right)^T \\ &\quad + \frac{\eta}{3} \left(\tilde{\nabla} \left(\tilde{\nabla}^T \hat{\mathbf{v}}^{n+1} \right) \right)^T - \frac{2}{3} \left(\tilde{\nabla}^T \hat{\mathbf{v}}^{n+1} \right) \left(\tilde{\nabla} \eta \right)^T, \end{aligned} \quad (3.33)$$

where $\eta = \eta_{\text{lam}}^n + \eta_{\text{turb}}^n$. Similar to the previous steps, the equation yields a large sparse linear system of equations. The solution for the preliminary velocity of the next time step $\hat{\mathbf{v}}^{n+1}$ is required to be corrected as it might not meet all constraints such that the divergence $\tilde{\nabla}^T \hat{\mathbf{v}}^{n+1}$ might not be correct [JEFFERIES ET AL. 2015].

To update the velocity and pressure, an implicit projection-type approach is applied by finding an additional correction term p_{corr}^{n+1} [CHORIN 1968, BROWN ET AL. 2001]. Thus, Equation (3.33) is modified as

$$\left(\mathbf{I} - \frac{\Delta t}{\varrho^{n+1}} \tilde{\Theta}^{n+1} \right) \mathbf{v}^{n+1} = \mathbf{v}^n - \frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} \hat{p} - \frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} p_{\text{corr}}^{n+1} + \Delta t \mathbf{g}. \quad (3.34)$$

Subtracting the two equations produces

$$\mathbf{v}^{n+1} - \hat{\mathbf{v}}^{n+1} - \frac{\Delta t}{\varrho^{n+1}} \tilde{\Theta}^{n+1} \left(\mathbf{v}^{n+1} - \hat{\mathbf{v}}^{n+1} \right) = - \frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} p_{\text{corr}}^{n+1}, \quad (3.35)$$

where applying the divergence operator yields

$$\left(\tilde{\nabla}^T \mathbf{v}^{n+1} \right) - \left(\tilde{\nabla}^T \hat{\mathbf{v}}^{n+1} \right) - \tilde{\nabla}^T \left(\frac{\Delta t}{\varrho^{n+1}} \tilde{\Theta}^{n+1} \left(\mathbf{v}^{n+1} - \hat{\mathbf{v}}^{n+1} \right) \right) = - \tilde{\nabla}^T \left(\frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} p_{\text{corr}}^{n+1} \right). \quad (3.36)$$

Here, the following term is assumed to be neglectable, noting that these constraints can always be achieved by properly adjusting the time step size [KUHNERT 2014]

$$\tilde{\nabla}^T \left(\frac{\Delta t}{\varrho^{n+1}} \tilde{\Theta}^{n+1} \left(\mathbf{v}^{n+1} - \hat{\mathbf{v}}^{n+1} \right) \right) \approx 0. \quad (3.37)$$

Thus, Equation (3.36) can be rewritten as

$$\tilde{\nabla}^T \left(\frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} p_{corr}^{n+1} \right) = - \left(\tilde{\nabla}^T \mathbf{v}^{n+1} \right) + \left(\tilde{\nabla}^T \hat{\mathbf{v}}^{n+1} \right), \quad (3.38)$$

where it is a Poisson-type equation to solve for the correction pressure p_{corr}^{n+1} . On the right hand side, the preliminary velocity $\hat{\mathbf{v}}^{n+1}$ is already evaluated. Furthermore, it is required that

$$\left(\tilde{\nabla}^T \mathbf{v}^{n+1} \right) \stackrel{!}{=} 0, \quad (3.39)$$

since the flow is considered to be incompressible for this study.

In order to couple the velocity and the pressure solutions in an implicit time integration, the penalty formulation introduced in KUHNERT 2014 is used. The numerical scheme for the velocity denoted as Equation (3.33) is enhanced by the correction pressure, and it is solved by incorporating with the scheme in Equation (3.38), which penalizes incorrect values of the velocity divergence. This is illustrated as

$$\begin{aligned} \left(\mathbf{I} - \frac{\Delta t}{\varrho^{n+1}} \tilde{\Theta}^{n+1} \right) \hat{\mathbf{v}}^{n+1} + \frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} p_{corr}^{n+1} &= \mathbf{v}^n - \frac{\Delta t}{\varrho^{n+1}} \tilde{\nabla} \hat{p} + \Delta t \mathbf{g}, \\ \left(\tilde{\nabla}^T \hat{\mathbf{v}}^{n+1} \right) - \tilde{\nabla}^T \left(\frac{\Delta t_{virt}}{\varrho^{n+1}} \tilde{\nabla} p_{corr}^{n+1} \right) &= \tilde{\nabla}^T \mathbf{v}^{n+1}, \end{aligned} \quad (3.40)$$

where Δt_{virt} is the virtual time step size, whose value can be flexible. If $\Delta t_{virt} = \Delta t$, it corresponds to an implicit Chorin projection [CHORIN 1968]. Theoretically, if $\Delta t_{virt} = 0$ is chosen, this would result in the exact solution. However, the linear system becomes ill-conditioned in this case, which can not be solved via an iterative solver in most of the cases [MICHEL ET AL. 2021]. Thus, it can be defined by using a coefficient

$$\Delta t_{virt} = K_{virt} \Delta t, \quad (3.41)$$

where $0.001 \leq K_{virt} \leq 0.1$ provides good conditioning of the linear system and yields a solution that is very close to the desired velocity divergence [JEFFERIES ET AL. 2015].

- Step 6. Update velocity and pressure

The velocity and dynamic pressure are updated according to the previous step given by [MICHEL ET AL. 2021]

$$\begin{aligned} \mathbf{v}^n &= \hat{\mathbf{v}}^{n+1} - \frac{\Delta t_{virt}}{\varrho^{n+1}} \tilde{\nabla} p_{corr}^{n+1}, \\ p_{dyn}^{n+1} &= p_{dyn}^n + p_{corr}^{n+1}. \end{aligned} \quad (3.42)$$

- Step 7. Turbulence

For the time integration step of turbulence, a singularity formulation of Equation (3.7) is first derived as [MICHEL ET AL. 2021]

$$\begin{aligned}
\frac{d}{dt} \left(\frac{k}{\varepsilon} \right) &= (C_{2\varepsilon} - 1) + C_\eta (1 - C_{1\varepsilon}) \left\| \tilde{\nabla} \mathbf{v}^T \right\|_M^2 \left(\frac{k}{\varepsilon} \right)^2 \\
&\quad + \frac{C_\eta (C_{1\varepsilon} C_{3\varepsilon} - 1)}{\rho Pr_{\text{turb}}} \frac{\partial \rho}{\partial T} (\mathbf{g} \cdot \tilde{\nabla} T) \left(\frac{k}{\varepsilon} \right)^2 \\
&\quad + \frac{1}{\rho} \tilde{\Delta}_{\eta^*} \left(\frac{k}{\varepsilon} \right), \\
\frac{d}{dt} \left(\frac{\varepsilon}{k} \right) &= (1 - C_{2\varepsilon}) \left(\frac{\varepsilon}{k} \right)^2 + C_\eta (C_{1\varepsilon} - 1) \left\| \tilde{\nabla} \mathbf{v}^T \right\|_M^2 \\
&\quad + \frac{C_\eta (1 - C_{1\varepsilon} C_{3\varepsilon})}{\rho Pr_{\text{turb}}} \frac{\partial \rho}{\partial T} (\mathbf{g} \cdot \tilde{\nabla} T) \\
&\quad + \frac{1}{\rho} \tilde{\Delta}_{\eta^*} \left(\frac{\varepsilon}{k} \right),
\end{aligned} \tag{3.43}$$

where

$$\begin{aligned}
\tilde{\Delta}_{\eta^*} \left(\frac{k}{\varepsilon} \right) &= \frac{\varepsilon \tilde{\Delta}_{\eta k} k - k \tilde{\Delta}_{\eta \varepsilon} \varepsilon}{\varepsilon^2}, \\
\tilde{\Delta}_{\eta^*} \left(\frac{\varepsilon}{k} \right) &= \frac{k \tilde{\Delta}_{\eta \varepsilon} \varepsilon - \varepsilon \tilde{\Delta}_{\eta k} k}{k^2}, \\
&\text{and} \\
\tilde{\Delta}_{\eta k} &= \tilde{\nabla}^T \left(\eta + \frac{\eta_{\text{turb}}}{\sigma_k} \tilde{\nabla} \right), \\
\tilde{\Delta}_{\eta \varepsilon} &= \tilde{\nabla}^T \left(\eta + \frac{\eta_{\text{turb}}}{\sigma_\varepsilon} \tilde{\nabla} \right).
\end{aligned} \tag{3.44}$$

When both $k, \varepsilon > 0$ for all $t^n \leq t \leq t^{n+1}$, numerical mean values can be represented as

$$\begin{aligned}
\left. \frac{k}{\varepsilon} \right|_{\text{mean}} &= \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \frac{d}{dt} \left(\frac{k}{\varepsilon} \right) dt, \\
\left. \frac{\varepsilon}{k} \right|_{\text{mean}} &= \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \frac{d}{dt} \left(\frac{\varepsilon}{k} \right) dt,
\end{aligned} \tag{3.45}$$

where these mean values are deployed to circumvent singularities in the $k - \varepsilon$ turbulence model discretization. Using the mean values, the standard $k - \varepsilon$ turbulence model equations are rewritten as [MICHEL ET AL. 2021]

$$\begin{aligned}\frac{dk}{dt} &= \frac{\tilde{\Delta}_{\eta k} k}{\varrho} - \frac{\varepsilon}{k} \Big|_{\text{mean}} k + C_{\eta} P_{\text{prb},k} \frac{k}{\varepsilon} \Big|_{\text{mean}} k, \\ \frac{d\varepsilon}{dt} &= \frac{\tilde{\Delta}_{\eta \varepsilon} \varepsilon}{\varrho} - C_{2\varepsilon} \frac{\varepsilon}{k} \Big|_{\text{mean}} \varepsilon + C_{1\varepsilon} C_{\eta} P_{\text{prb},\varepsilon} \frac{k}{\varepsilon} \Big|_{\text{mean}} \varepsilon,\end{aligned}\tag{3.46}$$

where

$$\begin{aligned}P_{\text{prb},k} &= \left\| \tilde{\nabla} \mathbf{v}^T \right\|_M^2 - \frac{1}{\varrho P r_{\text{turb}}} \frac{\partial \varrho}{\partial T} (\mathbf{g} \cdot \tilde{\nabla} T), \\ P_{\text{prb},\varepsilon} &= \left\| \tilde{\nabla} \mathbf{v}^T \right\|_M^2 - \frac{C_{3\varepsilon}}{\varrho P r_{\text{turb}}} \frac{\partial \varrho}{\partial T} (\mathbf{g} \cdot \tilde{\nabla} T).\end{aligned}\tag{3.47}$$

Thus, an implicit time integration scheme for the turbulent quantities is then denoted as

$$\begin{aligned}k^{n+1} - \frac{\Delta t \tilde{\Delta}_{\eta k} k^{n+1}}{\varrho} + \Delta t \frac{\varepsilon}{k} \Big|_{\text{mean}} k^{n+1} - \Delta t C_{\eta} P_{\text{prb},k}^{n+1} \frac{k}{\varepsilon} \Big|_{\text{mean}} k^{n+1} &= k^n, \\ \varepsilon^{n+1} - \frac{\Delta t \tilde{\Delta}_{\eta \varepsilon} \varepsilon^{n+1}}{\varrho} + \Delta t C_{2\varepsilon} \frac{\varepsilon}{k} \Big|_{\text{mean}} \varepsilon^{n+1} - \Delta t C_{1\varepsilon} C_{\eta} P_{\text{prb},\varepsilon}^{n+1} \frac{k}{\varepsilon} \Big|_{\text{mean}} \varepsilon^{n+1} &= \varepsilon^n.\end{aligned}\tag{3.48}$$

Here, the mean values are calculated analytically, assuming that the diffusion terms $\frac{1}{\varrho} \tilde{\Delta}_{\eta^*} \left(\frac{k}{\varepsilon} \right)$ and $\frac{1}{\varrho} \tilde{\Delta}_{\eta^*} \left(\frac{\varepsilon}{k} \right)$ are neglectable. Then, both equations in Equation (3.43) can be rearranged in the following form

$$\begin{aligned}\frac{dx}{dt} &= a - bx^2, \quad \text{where} \\ x &= \frac{k}{\varepsilon} \quad \text{or} \quad \frac{\varepsilon}{k}.\end{aligned}\tag{3.49}$$

The analytic solution of the above differential equation with $x_0 = \sqrt{\frac{a}{b}}$ is [MICHEL ET AL. 2021]

$$x^{n+1} = \begin{cases} x_0 \tanh \left(\Delta t \sqrt{ab} + \operatorname{arctanh} \left(\frac{x^n}{x_0} \right) \right), & x^n < x_0 \\ x_0, & x^n = x_0 \\ x_0 \coth \left(\Delta t \sqrt{ab} + \operatorname{arccoth} \left(\frac{x^n}{x_0} \right) \right), & x^n > x_0. \end{cases}\tag{3.50}$$

Using the analytic solution of the mean values, the entries of the sparse system are filled, and the system can be solved by using the chosen iterative solver. As the final step, the turbulent viscosity is given by [MICHEL ET AL. 2021]

$$\eta_{\text{turb}}^{n+1} = \varrho^{n+1} C_\eta \frac{(k^{n+1})^2}{\varepsilon^{n+1}}. \quad (3.51)$$

- Step 8. Concentration update

Similar to the temperature update procedure, a semi-implicit form for the vapor concentration, or vapor mass fraction, transport equation is illustrated as [MICHEL ET AL. 2021]

$$\begin{aligned} (\mathbf{I}_\Psi + \mathbf{D}_\Psi) \Psi^{n+1} &= \Psi^n, \quad \text{where} \\ \mathbf{I}_\Psi &= (\mathbf{I} + \Delta t \tilde{\nabla}^T \mathbf{v}^n), \\ \mathbf{D}_\Psi &= -\Delta t \tilde{\nabla}^T (D_{\text{eff}} \tilde{\nabla}). \end{aligned} \quad (3.52)$$

Note that the source terms generated by the evaporation for the temperature and concentration in Equations (3.31) and (3.52) are for now omitted. Details of the source terms are discussed in the following sections.

The interaction between the phases is defined by a surface-surface-coupling or a volume-volume-coupling scheme. Detailed explanations regarding the phase coupling schemes are discussed in the following section (Section 3.6.3).

Free surface treatments

First, the boundary conditions at free surface points can be given by a stress evaluation in the normal and tangential directions. This is done by equating the stresses at the free surface in the normal and tangential directions. It is given in 2D cases by [SUCHDE 2018]

$$\begin{aligned} \mathbf{t}^T \mathbf{S} \mathbf{n} &= 0, \\ \mathbf{n}^T \mathbf{S} \mathbf{n} &= p - p_0 - \sigma \kappa, \end{aligned} \quad (3.53)$$

where $\mathbf{t}$ is the tangential directional unit vector of the free surface, $\mathbf{n}$ is the outward pointing boundary normal unit vector, p_0 is the reference atmospheric pressure surrounding the free surface, and $\mathbf{S} = \mathbf{S}(\mathbf{v})$ is the stress tensor for velocity, σ is the surface tension, and κ is the local free surface curvature determined by geometrical formation. The Equation (3.53) is then simplified as

$$\begin{aligned} (2n^x t^x) \frac{\partial u}{\partial x} + (n^x t^y + n^y t^x) \frac{\partial u}{\partial y} + (n^x t^y + n^y t^x) \frac{\partial v}{\partial y} + (2n^y t^y) \frac{\partial v}{\partial x} &= 0, \\ (2(n^x)^2) \frac{\partial u}{\partial x} + (2n^x n^y) \frac{\partial u}{\partial y} + (2n^x n^y) \frac{\partial v}{\partial y} + (2(n^y)^2) \frac{\partial u}{\partial y} &= p - p_0 - \sigma \kappa \end{aligned}$$

(3.54)

This can be discretized in the following form

$$au_i + bv_i + c \sum_{j \in N_i} c_{ij}^x u_j + d \sum_{j \in N_i} c_{ij}^y u_j + e \sum_{j \in N_i} c_{ij}^x v_j + f \sum_{j \in N_i} c_{ij}^y v_j = g \quad (3.55)$$

such that it can be fed into the sparse system for the free surface boundary points.

Water mass transfer into vapor due to evaporation on the water side is not directly incorporated into the boundary conditions but imposed as a separate step after the standard free surface movement is calculated for both approaches – single-phase and multi-phase.

For each free surface point, its additional inward normal velocity is calculated from the given mass or volume change rate and the free surface area that the corresponding point represents as

$$\dot{m}_{\text{water}}'' = \frac{m}{At} = \frac{\rho V}{At}, \quad (3.56)$$

where $\dot{m}_{\text{water}}''$ is mass flux, A is surface area, m is mass, V is volume, and t is time. It should be noted that the double prime notation $\dot{m}''$ is used to specify that the mass transfer rate is expressed per unit area (i.e., mass flux). Thus, the local retrieve velocity magnitude of the free surface points in the inward normal direction is given by

$$v_{\text{retrieve}} = \frac{\dot{m}_{\text{water}}''}{\rho}, \quad \text{where} \quad (3.57)$$

$$\mathbf{v}_{\text{retrieve}} = v_{\text{retrieve}} \mathbf{n}.$$

The details regarding the mass transfer rate of flux will be covered in Section 3.6.2 and 3.6.3. Then, the point is shifted according to the calculated retrieve velocity and the current time step size. In the subsequent point cloud organization process, interior points that might have approached the free surface too closely will be combined with the free surface points to ensure the overall quality of the point cloud remains intact.

Given that every individual free surface point moves autonomously, depending on locally calculated evaporation rates, the present method inherently manages the free surface efficiently. Thus, the simulations effectively manage scenarios such as the water volume becoming disconnected during the ongoing mass transfer process or when discrete water volumes already exist from the initial state. Furthermore, the implementation contains a time-lapse factor, which can increase the speed of this additional surface movement due to evaporation, such that the evaporation effects can be sped up virtually and the overall simulation time for the dry-out can be reduced. This will be covered in Section 5.

Representative mass

Meshfree collocation methods like GFDMs are inherently not volume- or mass-conserving for the cases with the existence of free surfaces [SUCHDE ET AL. 2017]. However, it is important to correctly track the local and global water volume in mass transferring scenarios such as evaporation. Thus, a remedy to keep the mass conservation that is performed locally by explicitly distributing mass packages among the points should be provided. The total sum of all mass carrying points should represent the analytical mass that should be in the system. The corresponding mass is automatically redistributed when local (adaptive) refinement/coarsening is necessary [SUCHDE ET AL. 2023].

It should be highlighted that, in order to avoid the confusion coming from the terminology, the term “mass transfer” is used for the mass transport caused by physical phase change, whereas the term “mass migration” is used for the mass redistribution occurring in the GFDM point cloud organization.

First, the volume that is covered by each meshless point should be defined. There exist several methods, and the following geometric methods are commonly used in meshless approaches [SUCHDE ET AL. 2023]:

- The most straightforward method involves linking a node to the volume of a sphere with a specified diameter. This diameter may depend on factors such as neighborhood size, kernel width, or any other prescribed values. However, it has a significant drawback of inconsistency due to either large overlapping or uncovered volumes in the computation domain, as depicted in Figure 3.5a.
- The second method is to construct a global Voronoi tessellation of a point cloud from each point as visualized in Figure 3.5b. This method is proven to be consistent, but it is computationally extremely expensive, particularly when it needs to be reconstructed at each time step.
- The last method introduced in this study is local Voronoi tessellation. In this context, the volume for each point is given by the volume of the Voronoi cell locally defined with the support of neighboring points. These locally defined Voronoi cells are stitched together to generate a global tessellation, where a small overlap of the volume may occur as illustrated in Figure 3.5c. Nevertheless, the overlaps are trivial, and it is consistent [SUCHDE ET AL. 2017]. Moreover, this method is much faster than global tessellation for each time step.

Here, it should be noted that the actual tessellation is not computed and the Figure 3.5 is only for the visualization purpose.

If a point i with nearby points set NP_i is considered, the representative mass of the point at the first time step is denoted as

$$m_i(t=0) = \rho_i V_i, \quad (3.58)$$

where ρ_i is the density of the point, and V_i is the local volume notation, which is computed by a method explained in the previous paragraph. Furthermore, Δm_i is

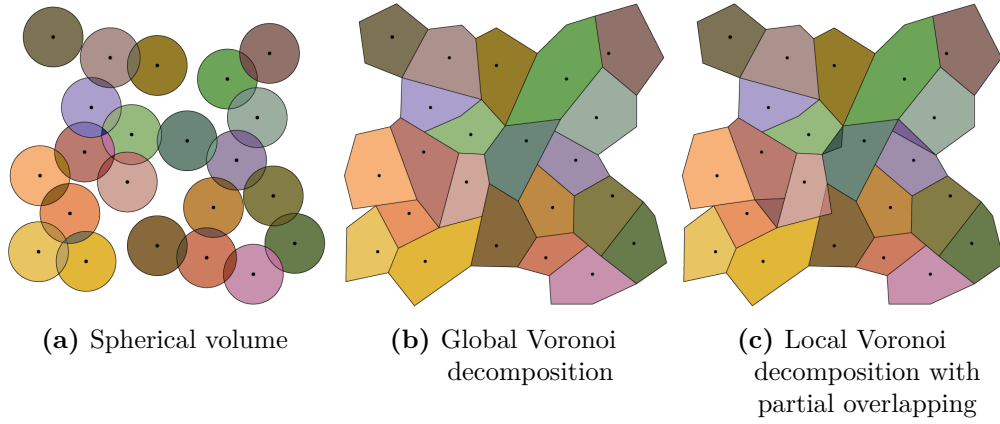


Figure 3.5: Different volume definition of point cloud. Adapted from [SUCHDE ET AL. 2023].

denoted for the change in representative mass in the next time step for a point i . Thus, a set of following conditions is to be fulfilled [SUCHDE ET AL. 2023].

1.) Constant total mass

Except for the inflow, outflow, and phase change (mass transfer) boundaries, the total mass should be constant as

$$\sum_{i=1}^{NP(t)} \Delta m_i = 0, \quad (3.59)$$

where $NP(t)$ is the total number of points in the computation domain. If any mass is added to a point, the amount of mass should be deducted from neighboring points such that

$$\Delta m_i = \sum_{j=1, j \neq i}^{NP(t)} \Delta m_{j \rightarrow i}. \quad (3.60)$$

2.) Local mass migration

A mass redistribution from points j to i should only occur if j is a direct neighborhood of i as

$$\Delta m_i = \sum_{j \in N_i, j \neq i}^{NP(t)} \Delta m_{j \rightarrow i}. \quad (3.61)$$

3.) Distance and mass dependency

The mass migration from a neighboring point j to i should diminish as the distance between the points increases. Furthermore, a greater amount of mass should be migrated from a neighbor with more mass, assuming all other conditions are identical. This helps prevent mass accumulation in specific points.

4.) Local computation

The computation of the redistribution should be a local procedure. As points move within a Lagrangian framework in each time step, and the addition/deletion of points also occurs in each time step, the mass migration procedure is executed at each time step. Opting for a localized calculation of the representative mass redistribution can substantially enhance the efficiency of the redistribution algorithm.

With the aforementioned conditions, the representative mass for each point can be written as

$$m_i + \sum_{j \in N_i, j \neq i}^{NP(t)} \Delta m_{j \rightarrow i} = m_i^{\text{target}}. \quad (3.62)$$

Here, the local mass change is computed for each cell with a neighborhood in both directions. Thus, the net change of mass of point i due to its neighbor j is calculated as

$$\Delta m_{ij} = \Delta m_{j \rightarrow i} - \Delta m_{i \rightarrow j}, \quad (3.63)$$

where $\Delta m_{j \rightarrow i}$ is calculated in the local computation of point i , and $\Delta m_{i \rightarrow j}$ is determined by the local calculation of point j . For the local redistribution process at each point, the following ansatz is introduced [SUCHDE ET AL. 2023]

$$\Delta m_{j \rightarrow i} = \gamma_i K_{ij} m_j, \quad (3.64)$$

where K_{ij} is transfer coefficient, and γ_i is a mass migration function. In order to meet the distance dependency rule, K_{ij} is based on the distance between the two points as

$$K_{ij} = \exp \left(-\alpha_K \frac{\|\mathbf{x}_j - \mathbf{x}_i\|^2}{\frac{h_i^2 + h_j^2}{2}} \right), \quad (3.65)$$

with a kernel width $\alpha_K = 2.0$. Thus, the mass migration function is obtained as

$$\gamma_i = \frac{\varrho_i V_i - m_i}{\sum_{j \in N_i, j \neq i} K_{ij} m_j}. \quad (3.66)$$

Using this mass function, which is computed and stored for each point, following mass adaptation or migration procedures are performed based on its own and neighbors' mass migration conditions.

- Addition of points

As explained in the previous section, in order to mitigate the artificial holes resulting from Lagrangian movement and when adaptive refinement is deployed, collocation points are added to the computation domain in this meshfree approach. A representative mass is allocated to a newly added point i through the execution of the mass adaptation

procedure. Since the initial mass of point i is zero, or $m_i = 0$, representing that the point did not have mass before the procedure, the mass function is given by

$$\gamma_i = \frac{\varrho_i V_i}{\sum_{j \in N_i, j \neq i} K_{ij} m_j}, \quad (3.67)$$

where N_i is the new neighborhood set for the new point.

- Deletion/Merging of points

Once two points approach each other too closely, one is removed, and the remaining point is relocated to the midpoint between the original two points. If point i is scheduled for deletion or is flagged as inactive, where no longer participating in the approximations is allowed, the mass redistribution procedure is employed with $V_i = 0$. This indicates that the deleted point should have zero volume. Consequently, the mass migration function becomes

$$\gamma_i = \frac{m_i}{\sum_{j \in N_i, j \neq i} K_{ij} m_j}. \quad (3.68)$$

- Boundaries

From the inflow boundary points, which are usually kept fixed in an Eulerian framework, new points are injected constantly into the domain along the inward normal direction. The mechanism of the new representative mass of these points is identical to the adding procedure explained previously. For a point on an outflow, the target representative mass in Equation (3.62) is determined by the mass flux across the boundary as

$$\frac{dm_i}{dt} \approx \frac{m_i^{\text{target}} - m_i}{\Delta t} = -\varrho_i (\mathbf{v} \cdot \mathbf{n}) A_i, \quad (3.69)$$

where $\mathbf{n}$ is the outward facing normal vector, and A_i is the area covered by the boundary point, which is computed by local tessellation. At the free surface boundary points, where the water mass transfer between the phase occurs, the volume and mass are corrected through mass transfer rate and the retrieve velocity explained in Section 3.6.1, 3.6.2, and 3.6.3. Then, the representative mass is redistributed accordingly in the following time step.

3.6.2 Single-phase approach for evaporation

The model used in the GFDM single-phase approach and the details of implementation to resolve evaporation physics are explained in this subsection.

Mass transfer rate

As MESHFREE can simulate free surfaces without the explicit presence of the air-phase, approximated mass transfer solutions for evaporation can be obtained with less computational effort using water-only single-phase simulations.

For the single-phase simulation, the convective mass transfer theory is applied in order to approximate the effects of the bulk air movement, as the air phase is not directly resolved. Thus, the mass transfer rate, or mass flux, is given by

$$\dot{m}_{\text{water}}'' = \varrho_{\text{air}} \alpha_{\text{mass}} \left(\Psi_{\text{vap}}^{\infty} - \Psi_{\text{vap}}^{\text{sat}}(T_{\text{water}}) \right), \quad (3.70)$$

where ϱ_{air} is the density of air, α_{mass} is the averaged mass transfer coefficient, $\Psi_{\text{vap}}^{\infty}$ is the ambient vapor concentration in air, and $\Psi_{\text{vap}}^{\text{sat}}(T_{\text{water}})$ is the saturation vapor concentration at the interface for the given temperature T_{water} . This equation is derived from the thermal-mass-analogy of Newton's law of cooling [ÇENGEL 2002].

It is not straightforward to obtain an exact, universally applicable mass transfer coefficient α_{mass} . Thus, several semi-empirical theories and equations have been developed to estimate it across various different scenarios exist [ÇENGEL 2002, SINGH & XU 1998]. Among them, one approximation can be obtained using Sherwood, Schmidt, and Reynolds number relations (Sh , Sc , and Re , respectively) by replacing the Nusselt and Prandtl numbers in the Nusselt equation as explained by [ÇENGEL & GHAJAR 2014, MEREDITH ET AL. 2011, INCROPERA ET AL. 2006]

$$\begin{aligned} Sh &= \frac{\alpha_{\text{mass}} L}{D_{\text{vap}}}, \\ Sc &= \frac{\nu}{D_{\text{vap}}} \quad (\approx 0.7 \text{ for vapor in air} - \text{used for this study}), \\ Re &= \frac{v_{\infty} L}{\nu}, \end{aligned}$$

where D_{vap} is the vapor mass diffusivity in air, ν is the kinematic viscosity, v_{∞} is the free stream velocity, and L is the length scale of the geometric surface, here the free surface of the water. Here, the Sherwood number estimation for forced convection over a flat plate is applied [ÇENGEL 2002], which is a similar scenario to the validation experiments presented in Section 4.1, leading to

$$Sh = \begin{cases} \frac{\alpha_{\text{mass}} L}{D_{\text{vap}}} = 0.664 Re^{1/2} Sc^{1/3}, & Re < 5 \times 10^5, \\ \frac{\alpha_{\text{mass}} L}{D_{\text{vap}}} = 0.037 Re^{4/5} Sc^{1/3}, & Re \geq 5 \times 10^5. \end{cases} \quad (3.71)$$

Utilizing this equation, the evaporation rate can be estimated and applied as a boundary condition at the free surface.

Energy balance

The exact amount of heat flux from air to water and the corresponding heat transfer coefficient cannot be obtained accurately in the water-only single-phase simulation, unlike in multi-phase simulations. Hence, achieving thermal equilibrium during a simulation run becomes challenging. Thus, it is assumed that the consumed latent heat at the free surface is compensated solely by the heat flux coming from air to the water bulk because equilibrium bulk water temperature, as well as air temperature, are imposed as the initial conditions and that the equilibrium thermal condition is sustained during the simulation. Moreover, according to the multi-phase simulations and the experiment done by [HISATAKE ET AL. 1995], it is observed that the temperature at the free surface of the water is merely 0.2–0.5°C lower than the bulk water temperature, which would have trivial effects on the results if taken into account.

Boundary conditions

In the water-only single-phase approach, where the air phase is not explicitly simulated, it is not required to define the limiting boundary elements for the air phase or air-box. Only the boundary elements in contact with the water phase should be specified as conventional no-slip for velocity, adiabatic walls for thermal conditions, and standard zero-gradient Neumann walls for pressure boundary conditions.

Here, the mass transfer rate is straightforwardly computed at the free surface, as explained in Section 3.6.2, and the corresponding mass is reduced by the method explained in Section 3.6.1, which is practically a negative source term at the boundary points.

3.6.3 Multi-phase approaches for evaporation

This subsection elaborates a detailed explanation of how the GFDM multi-phase approaches – for both surface-surface- and volume-volume-coupling – are implemented.

Surface-surface-coupling

For the surface-surface-coupling multi-phase simulations, an example of the initial domain discretization can be seen in Figure 3.4. The figure illustrates the distinct regions of the air and water phases. Points of both phases are present at the interface, as shown in Figure 3.4. With this approach, interface boundary conditions for each phase can be enforced. For a coupling between the phases across the interface, each interface point is associated with an *opposite* interface point of the other phase.

To enforce these conditions, the normal vector $\mathbf{n}$ is introduced at each interfacial point. This vector defines the normal coordinate to the interface and is critical for ensuring the coupling between the phases.

For example, when an interfacial point j^{water} of the water phase is considered, at each time step, this point is associated with a point i^{air} of the air phase, which is the interface air point closest to j^{water} in the direction of $\mathbf{n}$.

The implicit coupling scheme involves solving two phases independently based on the classical FPM framework, accompanied by additional conditions at the surface-surface interface.

Two phases are indicated with indices I and II, respectively. The surface-surface-coupling scheme can be written as [KUHNERT ET AL. 2017]

$$\left\{ \begin{array}{l} (p^{\text{I}}, \mathbf{v}^{\text{I}})(t^{n+1}) = \text{FPMsolver}(\Delta t; p^{\text{I}}(t^n), \mathbf{v}^{\text{I}}(t^n)), \\ (p^{\text{II}}, \mathbf{v}^{\text{II}})(t^{n+1}) = \text{FPMsolver}(\Delta t; p^{\text{II}}(t^n), \mathbf{v}^{\text{II}}(t^n)), \\ p^{\text{I}} = p^{\text{II}}|_{\text{interface}}, \\ \frac{\partial p^{\text{I}}}{\partial \mathbf{n}} = - \frac{\partial p^{\text{II}}}{\partial \mathbf{n}}|_{\text{interface}}, \\ \frac{\partial \mathbf{v}^{\text{I}}}{\partial \mathbf{n}} = - \frac{\partial \mathbf{v}^{\text{II}}}{\partial \mathbf{n}}|_{\text{interface}}, \\ \mathbf{v}^{\text{II}} = \mathbf{v}^{\text{I}}|_{\text{interface}}. \end{array} \right. \quad (3.72)$$

To determine a physical quantity of interest, for example, the vapor concentration gradient of the air phase near j^{water} , the corresponding value at i^{air} will be used. A similar concept of the opposite point is also used for the air phase to determine water phase quantities nearby.

Volume-volume-coupling

The underlying idea of the volume-volume-coupling is that the two phases only exchange required information by approximation from one phase to the other. In this context, only one phase models the complex free surfaces (water phase point cloud), while the other phase (air phase point cloud) overlaps more complex phase.

For the coupling, the Brinkman model is used [KUHNERT ET AL. 2017, SEIFARTH 2018]. A comparison of the initial point cloud organization of both the surface-surface-coupling, where no overlap is allowed, and the volume-volume-coupling with phase overlapping is depicted in Figure 3.6.

For the overlapping phase (Phase I or air in the current application), the conventional momentum conservation equation is extended to

$$\frac{d\mathbf{v}^{\text{I}}}{dt} + \frac{1}{\varrho} \nabla p^{\text{I}} = \frac{1}{\varrho} (\nabla^{\text{T}} \mathbf{S}^{\text{I}})^{\text{T}} + \mathbf{g} - \beta (\mathbf{v}^{\text{I}} - \mathbf{v}^{\text{II}}), \quad (3.73)$$

where $\nabla^{\text{T}} \mathbf{S}^{\text{I}}$ is the divergence of the stress tensor in phase I and $\mathbf{g}$ is the gravitational body force, assuming that the flow is incompressible ($\nabla^{\text{T}} \mathbf{v} = 0$) [KUHNERT 2014]. The

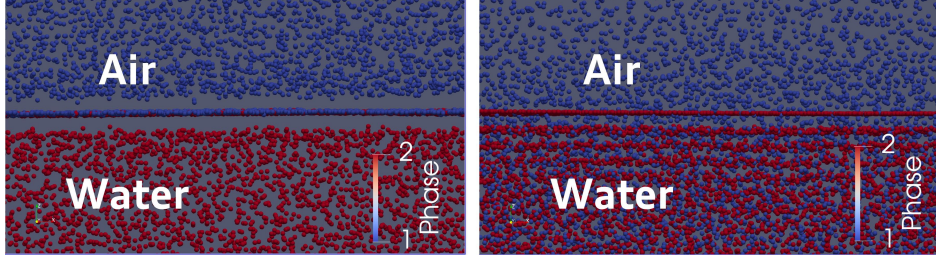


Figure 3.6: Point cloud organization examples of the non-overlapping surface-surface-coupling (left) and the overlapping volume-volume-coupling (right). Adopted from [LEE ET AL. 2024].

drag coefficient (β) and the reference velocity ($\mathbf{v}_{\rightarrow I}^{\text{II}}$) are determined by the other phase as the overlapping phase flows through a porous medium whose properties are defined by the other phase [KUHNERT ET AL. 2017, SEIFARTH 2018]. When there are no Phase II points near a Phase I point within the local search area, the flow remains unobstructed by the other phase at that particular location, resulting in a drag coefficient of zero for that point, i.e., $\beta = 0$. If a point in phase I finds a local neighboring point of phase II, or a bulk-like neighborhood for our specific case, the parameter of drag coefficient is assigned a properly large value, such as $\beta = 10^4$, at this specific location to model an impermeable medium.

The underlying physical model for the second phase (Phase II or water) aligns with the conventional conservation equations. The momentum equation of the second phase is formulated as follows:

$$\frac{d\mathbf{v}^{\text{II}}}{dt} + \frac{1}{\rho} \nabla p^{\text{II}} = \frac{1}{\rho} (\nabla^T \mathbf{S}^{\text{II}})^T + \mathbf{g}^{\text{II}}. \quad (3.74)$$

In the case of a bulk-like free surface formation, where phase II acts as an impermeable medium from phase I point of view, the stagnation pressure from phase I exerted on the local free surface of phase II is employed as the conventional fixed-value Dirichlet boundary condition [KUHNERT ET AL. 2017]:

$$p^{\text{II}}|_{\text{FS}} = \frac{1}{2} \rho^{\text{I} \rightarrow \text{II}} \left((\mathbf{v}_{\rightarrow \text{II}}^{\text{I}} - \mathbf{v}^{\text{II}}) \cdot \mathbf{n}^{\text{II}} \right)^2, \quad (3.75)$$

where the coupling terms are based on the projected or approximated values by neighboring phase I points.

Unlike in the surface-surface-coupling approach, the physical quantities of interest, such as the vapor concentration gradient, are not determined by an *opposite* interface point but by the projected value from the nearby other phase points. This approach makes it possible to approximate any required physical quantities of the other phase stably even if the free surface point cannot find a coupled *opposite* point in the surface-surface-coupling scenarios. Such situations could lead to a complete breakdown of the coupling conditions.

Mass transfer and thermal balance

In the multi-phase scenarios, the liquid mass is transferred into vapor by the force driven by the vapor concentration gradient in the vicinity of the interface in the air phase. Hence, the local mass transfer rate, or mass flux, $\dot{m}_{\text{water}}''$ can be calculated as

$$\dot{m}_{\text{water}}'' = \varrho_{\text{air}} D_{\text{vap}} \left. \frac{\partial \Psi_{\text{vap}}}{\partial \mathbf{n}} \right|_{\text{air,interface}}, \quad (3.76)$$

where ϱ_{air} is the density of air, D_{vap} is the diffusivity of vapor in air, and $\left. \frac{\partial \Psi_{\text{vap}}}{\partial \mathbf{n}} \right|_{\text{air,interface}}$ shows the normal-directional vapor concentration gradient at the interface. This equation is based on the Fick's law of diffusion, and it is assumed that the vapor concentration, or vapor partial pressure, always corresponds to the saturation concentration or saturation partial pressure at the interface for the given interfacial temperature [ÇENGEL 2002].

The water vapor concentration Ψ_{vap} , or water vapor mass fraction in air, with respect to the given condition, can be calculated as

$$\Psi_{\text{vap}} = \frac{M_{\text{vap}}}{M_{\text{air}}} \frac{p_{\text{vap}}}{p - p_{\text{vap}}} = 0.622 \frac{\varphi p_{\text{vap}}^{\text{sat}}}{p - \varphi p_{\text{vap}}^{\text{sat}}}, \quad (3.77)$$

where M_{air} , M_{vap} are the averaged molar masses of air and the molar mass of vapor, φ represents the relative humidity, $p_{\text{vap}}^{\text{sat}}$ is the saturation partial pressure of vapor at the given temperature, and p is the total pressure of air or the atmospheric pressure for the simplicity [KALINAY 2017]. $p_{\text{vap}}^{\text{sat}}$ at the given temperature can be obtained utilizing either the Arden Buck Equation or the Psychrometric Chart [SCHASCHKE 2014, BUCK 1981].

The effective diffusivity $D_{\text{vap,eff}}$ for vapor in air is defined as the combination of the laminar and turbulent diffusivity, expressed as

$$D_{\text{vap,eff}} = D_{\text{vap,lam}} + D_{\text{vap,turb}}. \quad (3.78)$$

The laminar diffusivity is given by [HILBRUNNER 2005]

$$\left[\frac{D_{\text{vap,lam}}}{\text{m}^2/\text{s}} \right] = 2.3056 \times 10^{-5} \frac{p_0}{p} \left(\left[\frac{T}{273 \text{ K}} \right] \right)^{1.81}, \quad (3.79)$$

where p_0 is the atmospheric pressure, p is the current pressure, and T is the absolute temperature. It should be noted that the leading coefficient is modified from the original version from the literature due to unit conversion from $\frac{\text{m}^2}{\text{h}}$ to $\frac{\text{m}^2}{\text{s}}$. In the current target applications, $\frac{p_0}{p}$ is effectively 1; thus, the laminar diffusivity solely depends on the temperature.

When the standard $k - \varepsilon$ turbulence model is adopted [MICHEL ET AL. 2021], the turbulent diffusivity is given by [VERSTEEG & MALALASEKERA 2007]

$$D_{\text{vap,turb}} = C_\eta \frac{k_{\text{air}}^2}{\varepsilon_{\text{air}}}, \quad C_\eta = 0.09, \quad (3.80)$$

where k is the turbulent kinetic energy and ε is the turbulent dissipation rate assuming a turbulent airflow.

Balancing thermal energy at the interface is crucial due to the consumption of energy – specifically the latent heat – during the mass transfer process. Therefore, the following subsequent thermal equilibrium equation at the interface is also introduced:

$$\lambda_{\text{water}} \left. \frac{\partial T}{\partial \mathbf{n}} \right|_{\text{water,interface}} + \dot{q}_{\text{air to water}}'' + \dot{q}_{\text{radiation}}'' = -\dot{m}_{\text{water}}'' \Delta h_{\text{evap}}, \quad (3.81)$$

where Δh_{evap} is the evaporation enthalpy or latent heat of the water evaporation ($2257.1 \left(\frac{\text{kJ}}{\text{kg}} \right)$ [CENGEL & GHAJAR 2014]), λ_{water} is the thermal conductivity of water, $\left. \frac{\partial T}{\partial \mathbf{n}} \right|_{\text{water,interface}}$ is the derivative of water temperature at the interface in inward normal direction, and $\dot{q}_{\text{air to water}}''$, $\dot{q}_{\text{radiation}}''$ are the heat flux from air to water and due to solar radiation, respectively. In this study, we do not consider solar radiation, i.e., $\dot{q}_{\text{radiation}}'' = 0$.

Boundary conditions

In the multi-phase approaches, defining boundary conditions for the air is necessary to limit the computational domain. This involves conceptualizing an air box with inlet boundary conditions that are identical to the ambient air conditions. Specifically, at the inlet, constant flow rate and temperature are enforced as conventional Dirichlet boundary conditions. Additionally, a specified constant ambient humidity or vapor partial pressure is defined in terms of vapor mass fraction, calculated using the Equations (3.77) in Section 3.6.3, serving as the inlet boundary condition. On the other hand, at the outlet, conventional zero-gradient Neumann boundary conditions for these variables are applied. Furthermore, for the pressure, standard Neumann zero-gradient conditions for the inlet are applied, while atmospheric fixed pressure values with Dirichlet conditions for the outlet boundary conditions are applied.

For other geometric elements, normal no-slip, adiabatic wall, and standard zero-gradient wall pressure conditions are imposed, with no vapor concentration interaction defined. On the water side, standard no-slip and adiabatic wall boundary conditions are defined for geometric elements in contact with the water phase.

The boundary conditions for the phase interface region, which is the most interesting part of the current study, should be specified explicitly in GFDM multi-phase approaches. Here, the mass and thermal transferring boundary conditions are defined for both phases.

The water mass reduction treatment at the free surface is basically identical to the boundary condition of the single-phase approach (see Section 3.6.2). The water mass is reduced based on the mass transfer rate calculated at the free surface point with the model described in Section 3.6.3. Based on the calculated mass transfer rate, the consumed latent heat is deducted with a negative heat flux source term at the water side boundary points.

For the surface-surface coupling, the desired physical quantities from the air side required for the correct mass- and heat-transfer calculation, such as vapor concentration gradient or temperature gradient, are obtained directly by communicating with the associated *opposite* interface point. The boundary points on the air side, however, maintain the saturated vapor concentration corresponding to the given interfacial temperature, functioning as a source term to supply vapor to the air phase. Moreover, the heat transfer between the phases, considering the temperature difference on each side, is also implemented in the boundary conditions for both sides.

On the other hand, in the volume-volume-coupling, a water interfacial point first searches for the neighboring air phase points within the search radius. Then, the desired quantities are interpolated in an indirect manner based on the values stored in the neighboring air points. As there are no explicit boundary points from the air point of view, the overlapping air points always have the saturated vapor concentration value at the given temperature, so these points operate as a source term for the vapor.

Resolution of the singularity issue

In GFDM approaches, the free surface points move inward with the retrieve velocity, which is computed based on the mass transfer rate, as previously explained.

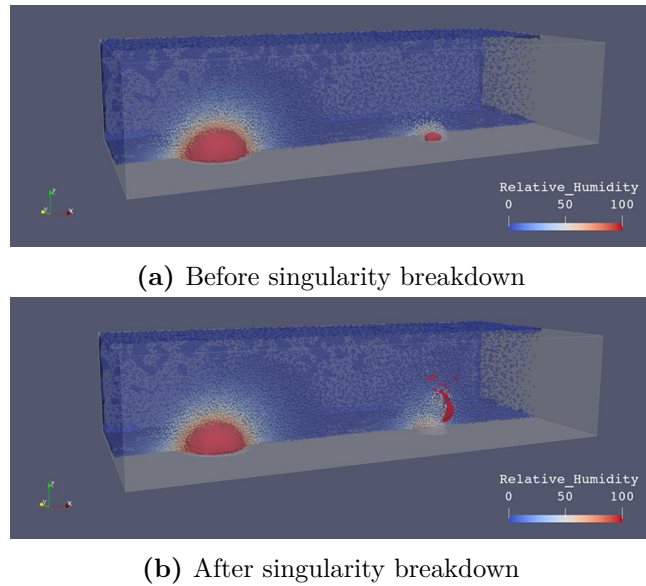


Figure 3.7: Singularity issue with GFDM approach when extremely small water volume is left. Water free surface is shown in 3D and air phase shows clipped image perpendicular to the water droplet.

Thus, when there is only an extremely small volume of water left, the simulation encounters a singularity scenario. Such cases produce free surface breakdowns and, eventually, the entire simulation becomes unstable, as illustrated in Figure 3.7.

In order to prevent the above critical scenario that may occur during the simulation runtime, every discrete water volume or droplet should be tracked cautiously and separately. If the volume of one or more water droplets becomes too small, i.e., below 10^{-7}m^3 , the simulation automatically detects the singularity risk and forces it to remove the corresponding water volume, so that the simulation does not crash and keeps running until the entire water volume in the computational domain fully evaporates.

3.7 Modeling and Implementations in FVM

A new model to simulate the water evaporation phenomenon is also implemented in FVM-based open source CFD code OpenFOAM developed by the ESI group. The base solver, which was extended with a new evaporation model, is called `icoReactingMultiphaseInterFoam`. It is a solver to solve N incompressible, non-isothermal immiscible fluids with phase-change and uses the VoF approach to capture phase interface [ESI GROUP 2024].

Here, the water phase is defined as a pure phase, whereas the air phase is defined as a multi-component phase model so that the air phase can contain both pure air (averaged physical properties of the combination of Nitrogen and Oxygen) and vapor within the phase. Each component in a multi-component would have fractional mass within the cell.

3.7.1 Finite Volume Method

The finite volume method (FVM) is a numerical approach that transforms the partial differential equations representing conservation laws across differential volumes into discrete algebraic equations over finite volumes. Similar to the finite difference (FD) or finite element method (FEM), the initial step of the solution process involves discretizing the geometric domain, which is also known as the meshing process. In the FVM, the domain is discretized into non-overlapping elements of finite volumes as shown in Figure 3.8. The partial differential equations are subsequently discretized or transformed into algebraic equations by integrating them over each discrete element. The system of algebraic equations is then solved to determine the values of the variable for each finite volume [MOUKALLED ET AL. 2016].

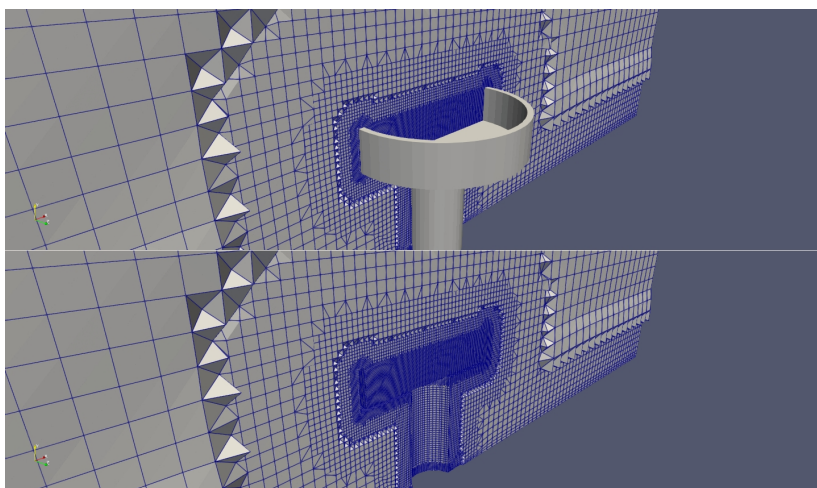


Figure 3.8: Domain discretization with non-overlapping finite volume elements example in 2D cross-section view with meshing around a vessel element. Upper figure includes the vessel geometry and the lower figure only shows generated mesh.

Domain discretization

First of all, the standard form of the transport equation for an arbitrary scalar property ϕ is shown as [JASAK 1996]:

$$\underbrace{\frac{\partial \varrho \phi}{\partial t}}_{\text{temporal derivative}} + \underbrace{\nabla^T(\varrho \mathbf{v} \phi)}_{\text{convection term}} = \underbrace{\nabla^T(\varrho D_\phi \nabla \phi)}_{\text{diffusion term}} + \underbrace{S_\phi(\phi)}_{\text{source term}}, \quad (3.82)$$

where ϕ is an arbitrary scalar function and D_ϕ is a diffusivity, noting that the equation is written in Eulerian form.

By integrating the Equation (3.82) over a finite volume element C , whose volume is V_C , the following integral form of the equation is obtained:

$$\int_{V_C} \frac{\partial \varrho \phi}{\partial t} dV + \int_{V_C} \nabla^T(\varrho \mathbf{v} \phi) dV = \int_{V_C} \nabla^T(\varrho D_\phi \nabla \phi) dV + \int_{V_C} S_\phi(\phi) dV. \quad (3.83)$$

The Gauss's theorem is described as

$$\begin{aligned} \int (\nabla \cdot \boldsymbol{\phi}) dV &= \oint \boldsymbol{\phi} \cdot \mathbf{n} dS, \\ \int (\nabla \phi) dV &= \oint \phi \mathbf{n} dS, \end{aligned} \quad (3.84)$$

where $\boldsymbol{\phi}$ is a continuously differentiable arbitrary vector field, $\mathbf{n}$ denotes the outward surface normal vector, dV represents the integration with respect to the volume, and dS the integration with respect to the surface. This theorem allows to establish a connection between the fluxes across the surface of any given volume element and the divergence operator acting on the volume element [HOLZMANN 2017].

By applying the Gauss's theorem, the Equation (3.83) is reformulated as

$$\int_{V_C} \frac{\partial \varrho \phi}{\partial t} dV + \oint_{\partial V_C} (\varrho \mathbf{v} \phi) \cdot \mathbf{n} dS = \oint_{\partial V_C} (\varrho D_\phi \nabla \phi) \cdot \mathbf{n} dS + \int_{V_C} S_\phi(\phi) dV, \quad (3.85)$$

where $\oint_{\partial V_C}$ is the surface integral over the volume V_C . The fundamental structure of the conservation equations previously stated is identical to the Equation (3.85) when it is rewritten in integral form.

The accuracy of the discretization method relies on the presumed variation of function ϕ in space and time around point C . Since an arbitrary function ϕ includes a diffusive term, which requires a second-order derivative in space, second-order or higher-order accuracy during the approximation is required. To obtain a second-order accuracy method using the Taylor series expansion, it is assumed that the function ϕ varies linearly from the point C along the space within the finite volume element as [JASAK 1996]:

$$\phi(\mathbf{x}) = \phi_C + (\mathbf{x} - \mathbf{x}_C) \cdot \nabla \phi_C, \quad \text{where} \quad \phi_C = \phi(\mathbf{x}_C). \quad (3.86)$$

Applying second-order approximation in space, the volumetric integral form in Equation (3.84) of the function ϕ is rewritten as

$$\begin{aligned}\int_{V_C} \phi dV &= \int_{V_C} [\phi_C + (\mathbf{x} - \mathbf{x}_C) \cdot \nabla \phi_C] dV \\ &= \phi_C \int_{V_C} dV + \left[\int_{V_C} (\mathbf{x} - \mathbf{x}_C) dV \right] \cdot \nabla \phi_C = \phi_C V_C,\end{aligned}\quad (3.87)$$

where the second integral is zero because the point C is the center of the control volume.

The surface integral form in Equation (3.84) is reformed as following

$$\begin{aligned}\oint_{\partial V_C} \phi \mathbf{n} dS &= \sum_f \left(\int_f \phi \mathbf{n} dS \right) \\ &= \sum_f \left(\int_f [\phi_f + (\mathbf{x} - \mathbf{x}_f) \cdot \nabla \phi_f] dS \right) = \sum_f \phi_f \mathbf{S}_f,\end{aligned}\quad (3.88)$$

where ϕ_f denotes the value of the function in the middle of the face f , and $\mathbf{S}_f$ is the outward face area vector.

Using this second-order approximation applied, the convection term in Equation (3.85) is now approximated as

$$\begin{aligned}\oint_{\partial V_C} (\rho \mathbf{v} \phi) \cdot \mathbf{n} dS &= \sum_f (\rho \mathbf{v} \phi)_f \cdot \mathbf{S}_f \\ &\approx \sum_f (\rho \mathbf{v})_f \phi_f \cdot \mathbf{S}_f = \sum_f F \phi_f,\end{aligned}\quad (3.89)$$

where $F = (\rho \mathbf{v})_f \cdot \mathbf{S}_f$ is the mass flux through the face. The quantities of the values at the face with subscription f are approximated by interpolating values from the cell centroid node values using a differencing scheme.

Generally, two differencing schemes are widely used for the convection terms – central differencing (CD) and upwind differencing (UD) schemes. The CD scheme evaluates the face value using a spatial linear interpolation between the computation nodes that share the considered face. Since the CD scheme inherently assumes that the function value changes linearly within the control volume C , it is considered as second-order method. Thus, discretization accuracy is not harmed. The face value is approximated as

$$\phi_f = f_x \phi_C + (1 - f_x) \phi_{NC}, \quad \text{where} \quad f_x = \frac{f \overline{NC}}{C \overline{NC}}, \quad (3.90)$$

where ϕ_{NC} is the node value of neighboring cell, f_x is defined as the ratio of distance $f \overline{NC}$ and $C \overline{NC}$.

In the UD scheme, the face value of ϕ is determined according to the flux direction of the convection flow as:

$$\phi_f = \begin{cases} \phi_C & \text{for } F \geq 0 \\ \phi_{NC} & \text{for } F < 0. \end{cases} \quad (3.91)$$

The UD is first-order accurate in space, and it is conditionally stable if the Courant-Friedrichs-Lewy condition is less or equal to one ($CFL \leq 1$).

The diffusion term is also discretized in a similar manner. By applying the second-order approximation, the diffusion term is reformulated as

$$\begin{aligned} \oint_{\partial V_C} (\varrho D_\phi \nabla \phi) \cdot \mathbf{n} dS &= \sum_f (\varrho D_\phi \nabla \phi)_f \cdot \mathbf{S}_f \\ &\approx \sum_f (\varrho D_\phi)_f (\nabla \phi)_f \cdot \mathbf{S}_f. \end{aligned} \quad (3.92)$$

Here, the surface normal gradient of ϕ to the face f ($(\nabla \phi)_f \cdot \mathbf{S}_f$) should be approximated. First, for the orthogonal face, where the face normal is parallel to the vector from cell centroid C to N , i.e. $(\mathbf{S}_f \parallel \mathbf{x}_{NC} - \mathbf{x}_C)$, the face normal gradient of ϕ is

$$(\nabla \phi)_f \cdot \mathbf{S}_f = \frac{\phi_{NC} - \phi_C}{|\mathbf{x}_{NC} - \mathbf{x}_C|} |\mathbf{S}_f|. \quad (3.93)$$

Second, for the non-orthogonal face, where the face normal vector is not aligned to the direction vector of two cell centroid points, a correction scheme should be deployed. One scheme among available schemes is called the over-relaxed approach. In this approach, the surface vector $\mathbf{S}_f$ is decomposed into two distinct vectors such that

$$\begin{aligned} \mathbf{S}_f &= \mathbf{S}_{f,\text{orth}} + \mathbf{\Delta}, \quad \text{where} \\ \mathbf{S}_{f,\text{orth}} &= \frac{(\mathbf{x}_{NC} - \mathbf{x}_C)}{(\mathbf{x}_{NC} - \mathbf{x}_C) \cdot \mathbf{S}_f} |\mathbf{S}_f|^2, \end{aligned} \quad (3.94)$$

where $\mathbf{S}_{f,\text{orth}}$ is parallel portion to the cell centroid direction vector and $\mathbf{\Delta}$ is difference vector. Then, the surface normal gradient is corrected as

$$\begin{aligned} (\nabla \phi)_f \cdot \mathbf{S}_f &= (\nabla \phi)_f \cdot (\mathbf{S}_{f,\text{orth}} + \mathbf{\Delta}) \\ &= (\nabla \phi)_f \cdot \mathbf{S}_{f,\text{orth}} + (\nabla \phi)_f \cdot \mathbf{\Delta} \\ &= \frac{\phi_{NC} - \phi_C}{|\mathbf{x}_{NC} - \mathbf{x}_C|} |\mathbf{S}_{f,\text{orth}}| + (f_x \nabla \phi_C + (1 - f_x) \nabla \phi_{NC}) \cdot \mathbf{\Delta}, \end{aligned} \quad (3.95)$$

where $\nabla \phi$ is approximated with linear interpolation for the $\mathbf{\Delta}$ part of the surface normal vector.

In the original transport equation, all terms that cannot be written as convection, diffusion, or temporal terms are considered as source terms [JASAK 1996]. The source term, denoted as $S_\phi(\phi)$ can be a general function of ϕ and is linearized as:

$$S_\phi(\phi) = S_u + S_p\phi, \quad (3.96)$$

where S_u and S_p can be functions of ϕ as well. The volume integral form of the source term is then given by

$$\int_{V_C} S_\phi(\phi) dV = S_u V_C + S_p V_C \phi_C. \quad (3.97)$$

Note that the discretization form of the source term should be determined based on the examination of its interaction with other terms and its influence on boundedness and accuracy [JASAK 1996].

Time integration

First, similar to spatial discretization, it is assumed that the function ϕ varies linearly in time in order to obtain a second-order accuracy [JASAK 1996]. Thus, employing Taylor series expansion, a linear temporal approximation of the time-dependent function ϕ is given by:

$$\phi(t + \Delta t) = \phi(t) + \Delta t \left(\frac{\partial \phi}{\partial t} \right)_t, \quad (3.98)$$

where the Taylor series expansion is truncated after the second term. This temporal discretization is, therefore, second-order accurate in time since the linear change in time yields the error scaling in second-order with the time step size Δt [JASAK 1996].

Next, the spatial integral form of the transport equation (Equation (3.83)) is reformed using temporal integration as

$$\begin{aligned} \int_t^{t+\Delta t} \left[\int_{V_C} \frac{\partial \phi}{\partial t} dV + \int_{V_C} \nabla^T (\rho \mathbf{v} \phi) dV - \int_{V_C} \nabla^T (\rho D_\phi \nabla \phi) dV \right] dt \\ = \int_t^{t+\Delta t} \left[\int_{V_C} S_\phi(\phi) dV \right] dt. \end{aligned} \quad (3.99)$$

Applying the equations derived for domain discretization, assuming that the control volumes do not change in time, the above equation is rewritten as a semi-discretized form [JASAK 1996]:

$$\begin{aligned} \int_t^{t+\Delta t} \left[\left(\frac{\partial \varrho \phi}{\partial t} \right)_C V_C + \sum_f F \phi_f - \sum_f (\varrho D \phi)_f (\nabla \phi)_f \cdot \mathbf{S}_f \right] dt \\ = \int_t^{t+\Delta t} (S_u V_C + S_p V_C \phi_C) dt. \end{aligned} \quad (3.100)$$

Here, using the Equation (3.98), the time derivative are calculated as

$$\left(\frac{\partial \varrho \phi}{\partial t} \right)_C = \frac{\varrho_C^{n+1} \phi_C^{n+1} - \varrho_C^n \phi_C^n}{\Delta t}, \quad (3.101)$$

where superscript n is the current time step, and $n+1$ is the next time step.

By substituting Equation (3.100) with the above equation, the equation is reformed as:

$$\begin{aligned} \int_t^{t+\Delta t} \left[\frac{\varrho_C^{n+1} \phi_C^{n+1} - \varrho_C^n \phi_C^n}{\Delta t} V_C + \sum_f F \phi_f - \sum_f (\varrho D \phi)_f (\nabla \phi)_f \cdot \mathbf{S}_f \right] dt \\ = \int_t^{t+\Delta t} (S_u V_C + S_p V_C \phi_C) dt. \end{aligned} \quad (3.102)$$

The discretization of the temporal derivative makes the values within time integral consistent over time across Δt . Moreover, it has become customary to neglect the change of the face values of ϕ and $\nabla \phi$ in time [PATANKAR 1980], making other terms such as convection, diffusion, and source terms are considered as temporally constant while integrating across Δt . Thus, the production of Δt during the time integration is eliminated on both sides, resulting in as following form:

$$\begin{aligned} \frac{\varrho_C^{n+1} \phi_C^{n+1} - \varrho_C^n \phi_C^n}{\Delta t} V_C + \sum_f F \phi_f - \sum_f (\varrho D \phi)_f (\nabla \phi)_f \cdot \mathbf{S}_f \\ = S_u V_C + S_p V_C \phi_C. \end{aligned} \quad (3.103)$$

The above-explained temporal discretization method is called the Euler method, which is first-order accurate, as the function values are assumed to be constant across Δt . Within the Euler method, there exist two different approaches: implicit and explicit. The method depends on the values that are used for ϕ or $\nabla \phi$ in non-temporal terms. The explicit Euler method uses the values of the old time step such that ϕ^n and $(\nabla \phi)^n$, whereas the implicit Euler method uses the values of the new time step, ϕ^{n+1} and $(\nabla \phi)^{n+1}$. For this study, the implicit Euler time discretization method, which is already

implemented in OpenFOAM, is deployed. The implicit Euler form of the generic transport equation is written by:

$$\begin{aligned} \frac{\varrho_C^{n+1} \phi_C^{n+1} - \varrho_C^n \phi_C^n}{\Delta t} V_C + \sum_f F \phi_f^{n+1} - \sum_f \left(\varrho D_\phi \right)_f (\nabla \phi)_f^{n+1} \cdot \mathbf{S}_f \\ = S_u V_C + S_p V_C \phi_C^{n+1}. \end{aligned} \quad (3.104)$$

As thoroughly explained in the previous section (Section 3.7.1), the required face values are calculated from the cell centroid values of surrounding cells using the selected differencing schemes in the above equation. Thus, rearranging the above equation yields an algebraic form for every cell as

$$a_C \phi_C^{n+1} + \sum_N a_{NC} \phi_{NC}^{n+1} = B_C, \quad (3.105)$$

where the values of a_C , a_{NC} , and B_C vary based on the physical problem being considered, the selected differencing schemes, and the chosen temporal discretization method. Since the value of ϕ_C^{n+1} depends on the values in the neighboring cells, the above algebraic form is assembled to generate a system of algebraic equations as

$$\mathcal{M} \phi = \mathcal{B}, \quad (3.106)$$

where $\mathcal{M}$ is a square matrix, whose diagonal entries are a_C and off-diagonal entries are a_{NC} . ϕ and $\mathcal{B}$ are column vectors that holds the values of variable ϕ and source term B for each cell. Generally, the $\mathcal{M}$ is a sparse matrix; only diagonal and a couple of off-diagonal entries are filled depending on the differencing schemes used. There are a number of available methods to solve this matrix in an iterative manner. In this study, the Gauss-Seidel smoother and geometric agglomeration multi-grid (GAMG) methods are mainly employed.

Pressure-velocity coupling procedure

As there is no explicit equation for pressure term in the fundamental governing equation of CFD, it is common to use a predictor-corrector iterative algorithm to solve the equation system or the generated matrix for FVM. The iterative algorithm deployed to solve the governing equations is based on the PIMPLE algorithm, which is basically a combination of the SIMPLE and PISO algorithms.

The SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm is used for the steady-state problems, where the resolution of the non-linear effects of the velocity is more important than the solution of the pressure field. In contrast, the PISO (Pressure-Implicit with Splitting of Operators) algorithm is suitable for transient simulations where a comprehensive solution of velocity-pressure coupling for each time step is required. The non-linear effects of velocity field are mitigated by employing small time steps or CFL Number smaller than 1 [PATANKAR 1980, ISSA 1986].

In the PIMPLE algorithm, apart from the original PISO inner loop, the momentum equation is placed inside the SIMPLE outer loop, where the momentum balance is recalculated many times since the non-linear effects of the velocity are more significant in transient simulations. Thus, the transient simulation runs stably even with larger time step sizes ($CFL > 1$).

The overview of the PIMPLE algorithm is shown in Figure 3.9.

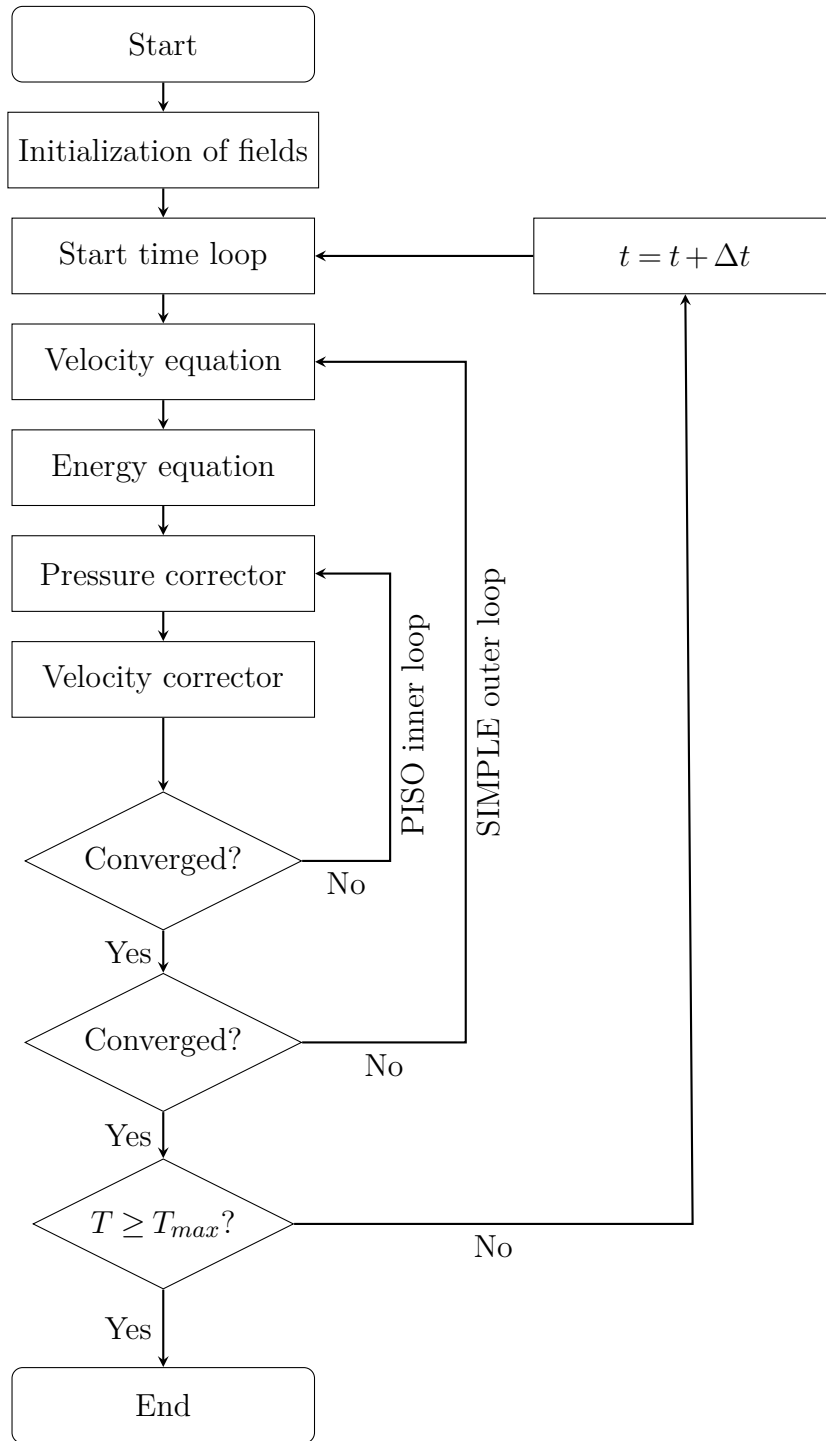


Figure 3.9: PIMPLE algorithm flow chart.

3.7.2 Volume of Fluid (VoF) model

One of the most widely used methods to model multiphase flows in FVM-based implementation is the Volume of Fluid model (VoF), originally proposed by HIRT & NICHOLS 1981. The VoF method tracks the phase interface on a stationary mesh by employing a tracking variable α , which represents the fraction of the traced volume V_i compared to the cell volume V :

$$\alpha_i = \frac{V_i}{V}. \quad (3.107)$$

Based on the values of α -field, each cell in the computation domain can be categorized into the following phases:

$$\alpha = \begin{cases} 0 & \text{in the gaseous phase} \\ 0 < \alpha < 1 & \text{in cells containing a part of the interface} \\ 1 & \text{in the liquid phase,} \end{cases} \quad (3.108)$$

where the example α field of a two-phase flow with the phase interface is illustrated in Figure 3.10.

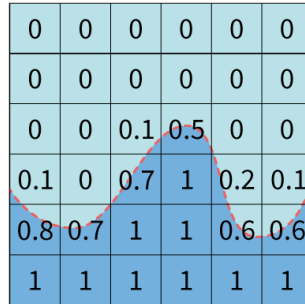


Figure 3.10: Example of the α field representation of each cell in two-phase flow.

For every cell, the volume fractions should sum up to 1 as, when each phase holds its own phase fraction α field [MOLTRECHT 2016]:

$$\sum_i \alpha_i = 1. \quad (3.109)$$

The α transport equation in original form is [SCHLOTTKE & WEIGAND 2008]

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{v}) = 0, \quad (3.110)$$

where no mass transfer between the phases is defined. When the mass transfer rate, which will be explained in the next section, is imposed, source and sink terms should be added.

The material properties ζ of the mixture phase such as dynamic viscosity η , density ϱ , heat capacity c_v , or thermal conductivity λ are calculated with a volume averaged value as:

$$\zeta = \alpha \zeta_1 + (1 - \alpha) \zeta_2, \quad \text{where } \zeta \in [\eta, \varrho, c_v, \lambda], \quad (3.111)$$

noting that the mass averaged isobaric heat capacity $\left(c_p = \frac{\alpha_1 \varrho_1 c_{p,1} + (1 - \alpha_1) \varrho_2 c_{p,2}}{\varrho}\right)$ can be used depending on the applications.

In the VoF model, a single momentum equation is solved for the mixture phase. In order to correct the pressure gradient term in the momentum equation, the pressure is modified to remove the hydrostatic component as

$$p_{rgh} = p - \varrho \mathbf{g} \cdot \mathbf{x}, \quad (3.112)$$

where $\mathbf{g}$ is the gravitational force and $\mathbf{x}$ is the position vector [RATTNER & GARIMELLA 2018].

Moreover, surface tension force is incorporated into a source term defined as

$$\mathbf{S}_\sigma = \sigma \nabla^T \left(\frac{(\nabla \alpha)}{|\nabla \alpha|} \right) \nabla \alpha, \quad (3.113)$$

where σ is the surface tension [KISSLING ET AL. 2010].

The resulting momentum equation can be written as

$$\frac{\partial}{\partial t} (\varrho \mathbf{v}) + \nabla^T (\varrho \mathbf{v} \otimes \mathbf{v}) - \nabla^T [\eta (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)] = -\nabla p_{rgh} - \nabla \varrho \mathbf{g} \cdot \mathbf{h} + \mathbf{S}_\sigma. \quad (3.114)$$

3.7.3 Multi-component mixture model

Apart from the VoF model, which defines the immiscible phase mixture flow (air and water), another model to resolve the vapor flow behavior in air phase is required. This is achieved with the multi-component model. In this model, different species with different thermo-physical properties are defined as components of one phase. Specifically, air as an inert species and vapor as a transporting species are defined for the computation.

In the VoF, which is modeled for immiscible mixture flow with an explicit interface between the phases, the physical properties are only volume averaged at interface cells, where both phases can simultaneously exist (as illustrated in Equation (3.111)). However, unlike the VoF, the multi-component mixture is for miscible species without interface.

Thus, every single cell within the air phase contains fractional values of each species, more specifically, mass fraction or concentration. The physical properties of each cell are calculated based on this mass fraction of species. The vapor mass fraction under the given condition in water can be calculated with Equation (3.77).

Based on the mass fraction, physical properties such as density and specific heat are calculated under the given temperature as

$$\varrho = \Psi_{\text{vap}} \varrho_{\text{vap}} + (1 - \Psi_{\text{vap}}) \varrho_{\text{air}} \quad \text{and} \quad c_p = \Psi_{\text{vap}} c_{p,\text{vap}} + (1 - \Psi_{\text{vap}}) c_{p,\text{air}}, \quad (3.115)$$

where other physical properties such as laminar viscosity (η) and laminar Prandtl number (Pr) assumed to remain constant.

The vapor transport equation within the air phase in Eulerian form, which is derived from Equation (3.10), is written as

$$\frac{\partial \Psi_{\text{vap}}}{\partial t} + \nabla^T (\Psi_{\text{vap}} \mathbf{v}) = \nabla^T (D_{\text{vap,eff}} \nabla \Psi_{\text{vap}}) + S_{\text{vap}}. \quad (3.116)$$

It should be noted that the diffusion term ($\nabla^T (D_{\text{vap,eff}} \nabla \Psi_{\text{vap}})$), which has a significant impact on the resulting mass fraction field, is missing in the OpenFOAM implementation. Thus, the diffusion term is included in the current study. A detailed explanation regarding the effective diffusivity of vapor ($D_{\text{vap,eff}}$) is already discussed in Section 3.6.3. Combining the entire partial differential equations to be solved introduced, the workflow of the comprehensive PIMPLE solver is presented in Figure 3.11. A detailed explanation regarding the source term S_{vap} is present in following sections (Section 3.7.4).

3.7.4 Mass transfer and thermal balance

The mass transfer rate principle in FVM is basically identical to the one used in the GFDM multi-phase approach as explained Section 3.6.3. Thus, the local area-specific mass source of vapor is driven by the vapor concentration gradient expressed as [CHEN ET AL. 2018, ÇENGEL 2002]:

$$\dot{m}_{\text{water}}'' = \varrho_{\text{air}} D_{\text{vap}} \left. \frac{\partial \Psi_{\text{vap}}}{\partial \mathbf{n}} \right|_{\text{air,interface}}, \quad (3.117)$$

noting that this equation is identical to the mass transfer equation explained in Section 3.6.3 – Equation (3.76). In the VoF approach, the above-stated mass transfer rate per area should be approximated into cell-wise mass transfer rate, $\dot{M}_{\text{water}}''$, as [SCHLOTTKE & WEIGAND 2008, SOH ET AL. 2016, MOLTRECHT 2016]:

$$\dot{m}_{\text{water}}'' \approx \dot{M}_{\text{water}}'' = \varrho_{\text{air}} D_{\text{vap}} |\nabla \alpha_{\text{water}}| V_C \nabla \Psi_{C,\text{vap}}. \quad (3.118)$$

Here, the interfacial area between the phases is approximated by using the area density function, $|\nabla \alpha|$. The resulting interfacial area is then calculated as, $\int |\nabla \alpha| dV = A_{\text{int}}$ [SOH ET AL. 2016, HARDT & WONDRA 2008, GUO ET AL. 2014]. The vapor

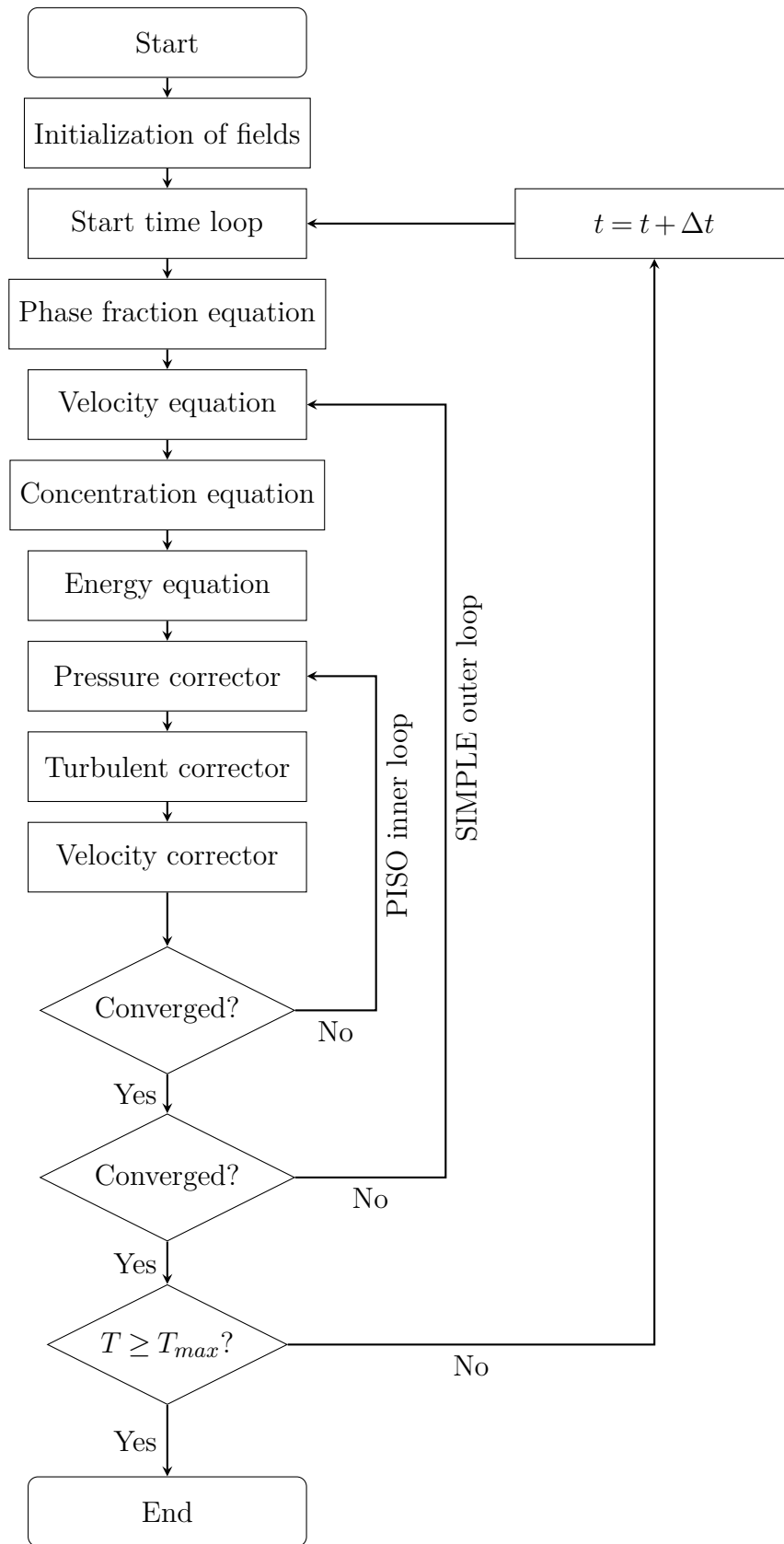


Figure 3.11: PIMPLE algorithm flow chart with comprehensive equation set.

concentration gradient at interfacial cell, $\nabla \Psi_{C,\text{vap}}$, can be calculated using following relation [MOLTRECHT 2016]:

$$\nabla \Psi_{C,\text{vap}} = \nabla \left(\alpha_{\text{water}} \Psi_{C,\text{vap}}^{\text{sat}} + \alpha_{\text{air}} \Psi_{C,\text{vap}} \right). \quad (3.119)$$

The cells completely filled with water phase are set to the saturated vapor mass fraction, whereas cells with air are set to the actual vapor mass fraction within the cells. Therefore, the cells located in the interfacial region, $(0 < \alpha < 1)$, take the interpolated value. One drawback of this approach is that the sharp interface representation in α -field should be kept in order to obtain accurate gradient computation [MOLTRECHT 2016].

This calculated cell-wise mass transfer rate is then fed into the continuity equation. The sink term with the corresponding mass is added in the continuity equation of the water phase and the source term in the air phase, more specifically, a source term for the vapor component. Likewise, a sink term in the α transport equation should be added as

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{v}) = - \frac{\dot{m}_{\text{water}}''}{\rho_{\text{liquid}}}. \quad (3.120)$$

Note that a sink term is added since the $\alpha = 1$ means liquid phase, and the mass transfer rate term is divided by the density as alpha is a volumetric representation.

The evaporation enthalpy or latent heat of vaporization consumed during the evaporation is then fed into the energy equations for each phase as sink terms. The actual amount dissipated, $\dot{m}_{\text{water}}'' \Delta h_{\text{evap}}$, is divided into half and then fed into the energy equations of each phase for simplicity. Thus, the thermal balance at the interface is achieved in the solving process.

3.7.5 Boundary conditions

The desired normal directional constant velocity and temperature with conventional fixed-value Dirichlet boundary conditions (BCs) are imposed at the inlet. Furthermore, as the VoF model is employed, α values should also be imposed as fixed-value Dirichlet BCs such as $\alpha_{\text{gas}} = 1$ and $\alpha_{\text{liquid}} = 0$, assuming no water is added to the evaporation simulation. In the air phase, the values for the two components (gas_{air} and gas_{vap}) are defined as Dirichlet BC, given that the mass fraction is properly calculated from the relative humidity at the given ambient temperature (Equation (3.77)). The pressure at the inlet is defined as standard zero-gradient Neumann BC.

For the outlet region, all the field variables that have fixed-value Dirichlet BC at the inlet (velocity, temperature, α^* , and gas^*) have conventional zero-gradient Neumann BCs. On the other hand, the pressure is imposed as a fixed-value Dirichlet BC with atmospheric pressure.

For any other geometries, no-slip for the velocity (Dirichlet), adiabatic wall (Neumann), and conventional zero-gradient pressure conditions are defined. α^* and gas^* fields also have zero-gradient Neumann BC such that no interaction with the wall is imposed

In the FVM approach, the behavior of the phase interface is resolved automatically via the VoF model with mass transfer implementation. Thus, explicit phase interface BC definitions for the field variables are not required, unlike in GFDM approaches.

4 Validation with a water vessel in a channel geometry

(The majority of the contents in this chapter is already published in journal articles [LEE ET AL. 2023a, LEE ET AL. 2024] and conference articles [LEE ET AL. 2022a, LEE ET AL. 2023c, LEE ET AL. 2022c].)

A series of experiments were conducted under different ambient conditions in order to validate the newly developed evaporation model in terms of the evaporation rate. In the designed experiment, three atmospheric variables – ambient air temperature, ambient air humidity, and airflow rate – that highly affect the evaporation rate were varied.

4.1 Experimental setup

The schematic of the validation experiment is shown in Figure 4.1. First of all, a channel of length 35cm with a cross-section of 14cm $\times$ 14cm was constructed in order to generate constant airflow by adjustable exhaust fans located at the outlet of the built channel. Four EBM Papst 8212 JN exhaust fans were placed at the channel end, as described in Figure 4.2. At the channel inlet, a coarse mesh plate (approximately 3cm $\times$ 3cm) and a fine mesh fabric (less than mm scale) were placed back-to-back as shown in Figure 4.3. Thus, turbulent effects were minimized, and constant inlet velocities were obtained. Second, a glass petri dish with an inner diameter of 80mm was installed as a water reservoir in the middle of the channel and on top of a metal cylinder of height 35mm and with a diameter of 50mm as depicted in Figure 4.4. In this water vessel, approximately 40g of water is initially deposited. The mass difference between the initial state and the remaining water mass after the experiment was measured to determine the evaporated water amount (with a scale accuracy of 10mg). This, coupled with the experiment duration, allowed the determination of the evaporation rate.

Three temperature/humidity sensors were installed along the channel, as in Figure 4.4. The sensor located closest to the inlet measured the inlet air temperature (with an accuracy of 0.5°C) and humidity (with an accuracy of 1.8%). These values were then used as inlet boundary conditions for the corresponding simulations.

The middle and outlet sensors were employed to observe the humidity distribution change caused by the evaporation from the water source. Lastly, a thermocouple inside the water vessel is placed to measure the temperature of the water body in an equilibrium state. These measurements were also used as initial water temperature conditions in the simulations. The entire channel setup was placed in a 1,000 liter climate chamber

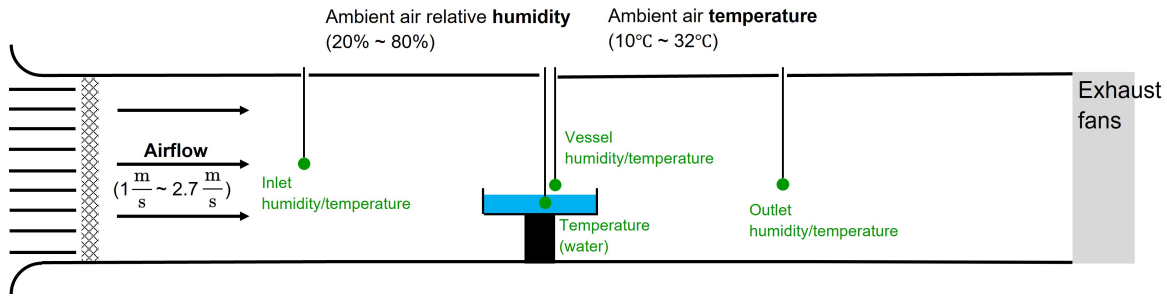


Figure 4.1: Schematic view of the evaporation rate measurement experiment.

Detailed dimensions of the actual experiment geometry are demonstrated in Section 4.1 as well as in Figure 4.6. Adopted from [LEE ET AL. 2023a].

(Weiss WK1 1000), as shown in Figure 4.5. Thus, the ambient air temperature and humidity inside the channel can be controlled as desired. The airflow rates generated by the four exhaust fans were measured with a flowmeter (with an accuracy of $0.1 \frac{\text{m}}{\text{s}}$) that was placed behind the inlet mesh structure inside the channel. Each flow rate was generated with a fixed voltage and current imposed by a voltage/current regulator on the exhaust fans.

The target conditions for the different experiment runs are shown in the following list. Note that the conditions in actual measurements are not exactly identical to the target values but show slight deviations, as the climate chamber is subject to inherent inaccuracies that cause discrepancies between the set and achieved conditions. For each experiment run, the actually measured values are described in the validation results comparisons. It should also be noted that the maximum airflow is set not to generate any wavy motion on the water surface, which causes inaccurate evaporation rate measurements.

- Airflow: $1.0 \frac{\text{m}}{\text{s}}$, $1.8 \frac{\text{m}}{\text{s}}$, and $2.7 \frac{\text{m}}{\text{s}}$
- Ambient air temperature: 10°C , 20°C , and 32°C
- Ambient air relative humidity: 20 % (30 % for 10°C), 40 %, 60 %, and 80 %

A total of 36 experiment rounds were conducted, all for an experiment duration of 90 minutes. It should be noted that a relative humidity of 30 % was used for the 10°C cases, as achieving the target value of 20 % relative humidity proved to be very difficult, despite being set as the desired condition.

The experimental results will be discussed in conjunction with the numerical results in the following comparison section, as they are presented in the subsequent figures.

4.2 Numerical simulation results

Both FVM and GFDM simulations are performed using a CAD geometry that is constructed to match the experimental setup described in Section 4.1 as in Figure 4.6.

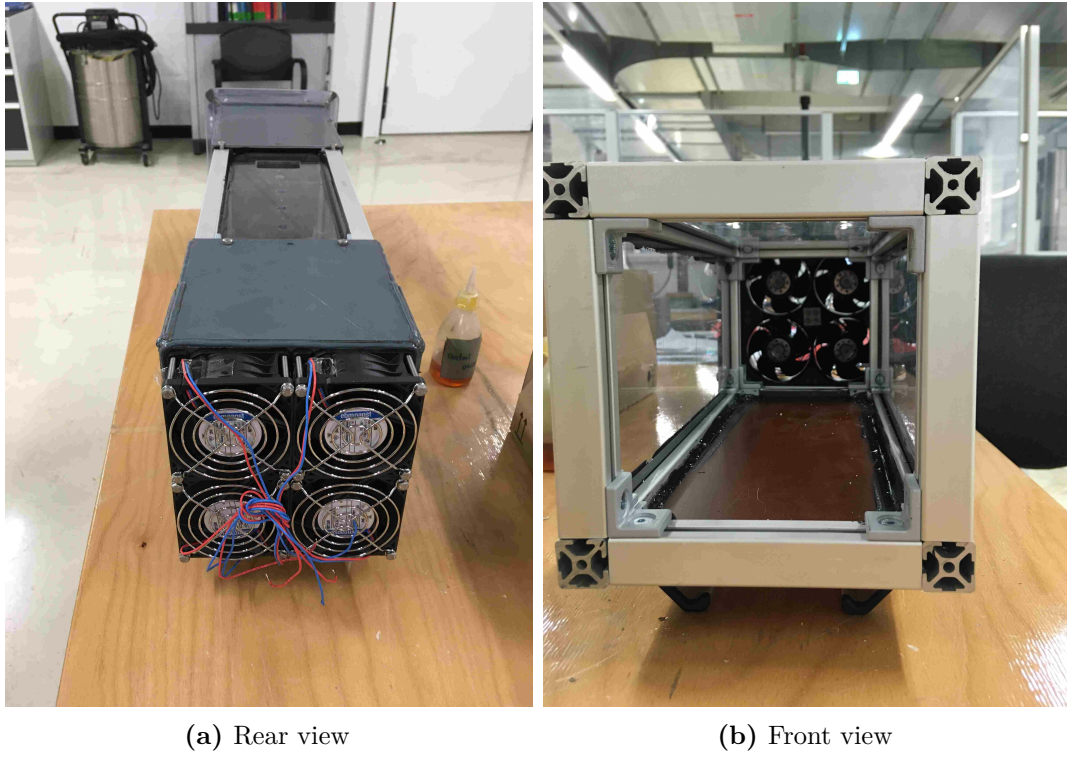


Figure 4.2: Experimental setup: Four EBM Papst 8212 JN axial fans at the channel outlet to generate constant airflow. Adopted from [LEE ET AL. 2023a].

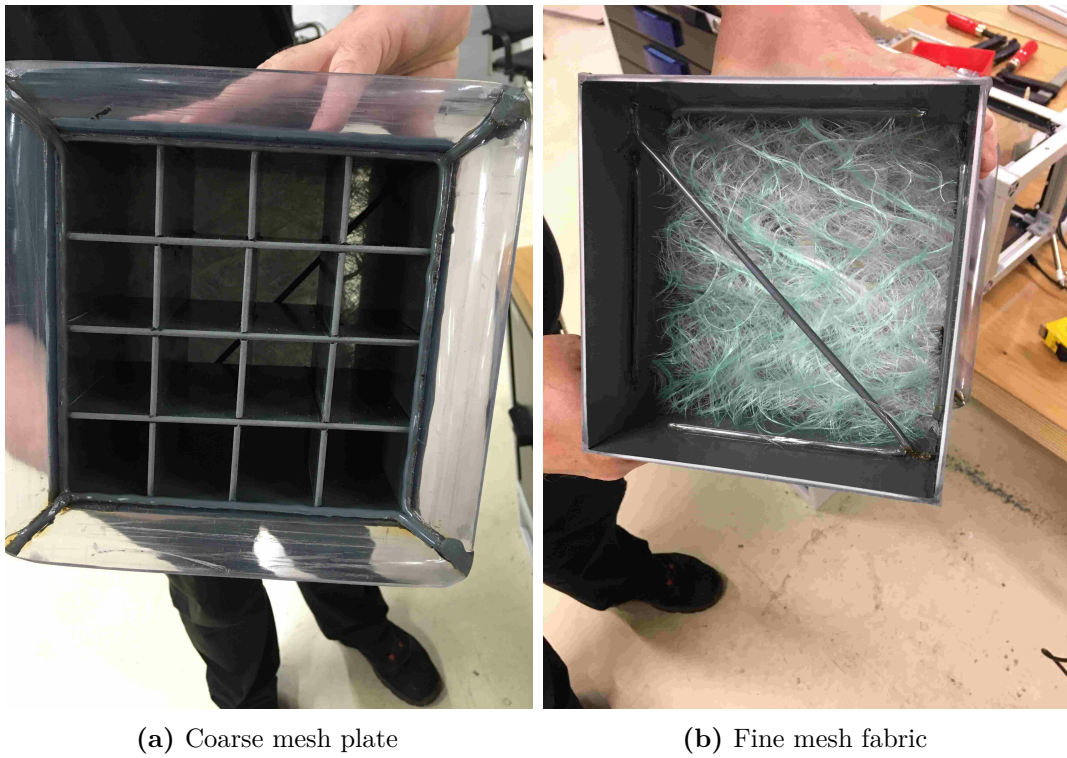
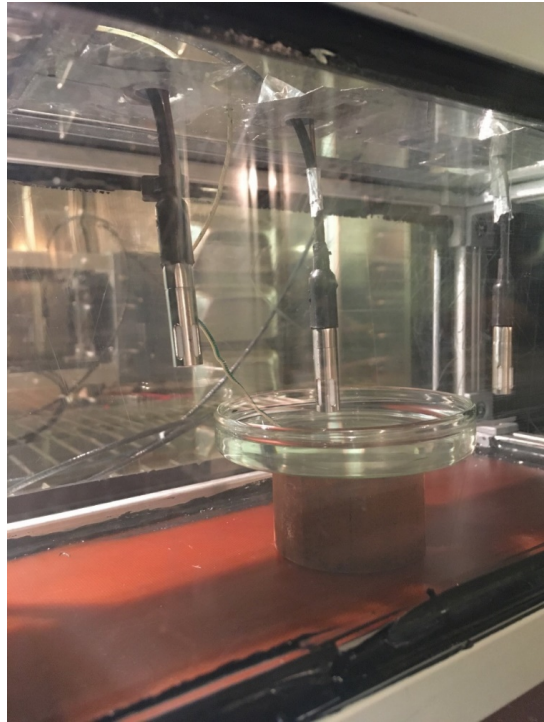


Figure 4.3: Experimental setup: Mesh structures at the channel inlet to reduce turbulence. Adopted from [LEE ET AL. 2023a].



(a) Water vessel placed in the middle of the channel



(b) Temperature/humidity sensors

Figure 4.4: Experimental setup: Structure inside the channel. Adopted from [LEE ET AL. 2023a].



(a) Complete view of the channel



(b) Channel placed inside the climate chamber

Figure 4.5: Experimental setup: Channel and climate chamber. Adopted from [LEE ET AL. 2023a].

Here, the ambient air temperature, relative humidity, and airflow rate conditions listed for the experiments are used for the simulations' initial and boundary conditions. In each simulation case, the required time-step size is automatically calculated with CFL conditions with the CFL number of 0.2. The resulting time-step sizes are in the order range from 10^{-4} to 10^{-5} s depending on the inlet velocities and the resulting velocity field changes over time within a simulation run.

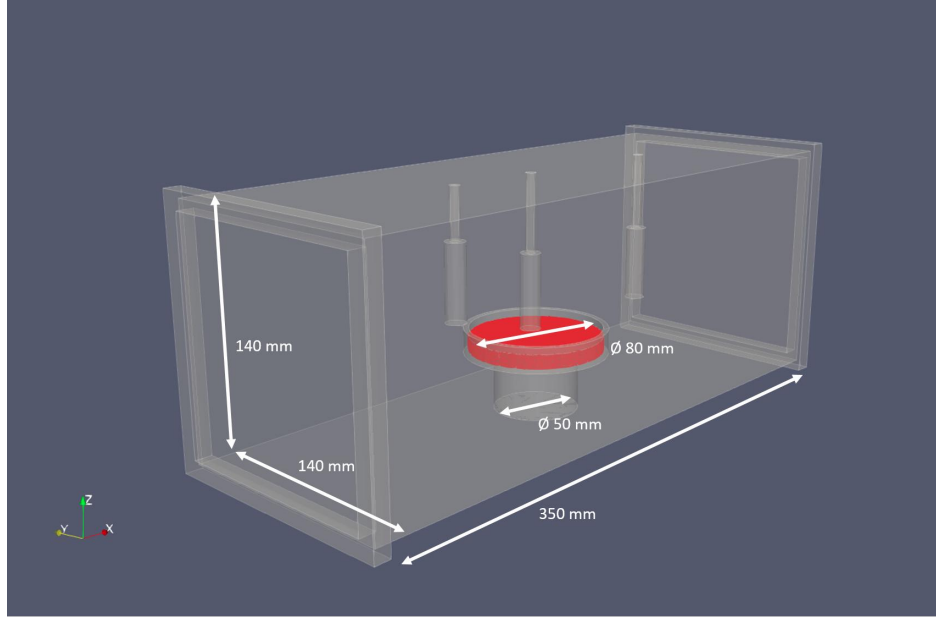


Figure 4.6: Bounding geometry matching the experimental setup (channel, sensors, and vessel). The red-colored region indicates the initial water mass in the vessel. Adopted from [LEE ET AL. 2023a].

4.2.1 OpenFOAM results

First, numerical simulations with the FVM-VoF method are performed. The 3D mesh overview generated from the CAD geometry (Figure 4.6) using **snappyHexMesh** tool is shown in Figure 4.7, noting that the mesh around the phase interface region is highly refined in order to correctly capture the phase interface as well as the evaporation phenomena. To obtain a mesh that is sufficient for the validation, mesh independency studies are conducted, which is to be discussed in hereinafter in this section.

With the generated mesh, the initial state of the water-air phases is defined with **setFields** utility in OpenFOAM as depicted in Figure 4.8. The ambient atmospheric conditions, such as air temperature, flow rate, and relative humidity, are then imposed as boundary conditions at the inlet (and also for the initial internal fields).

Quasi-steady state evaporation rate

In Figure 4.9, the resulting relative humidity profiles at 2s and 20s are shown for the simulation run with $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 40.6% relative

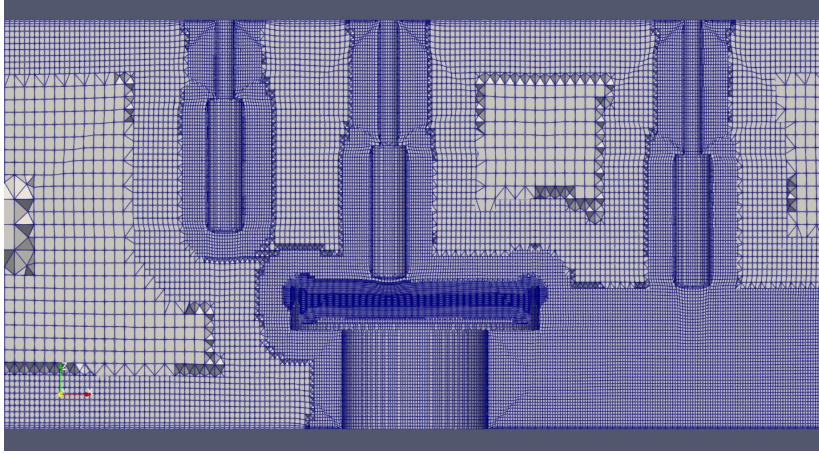


Figure 4.7: Mesh pre-processing overview for FVM simulation for the validation.

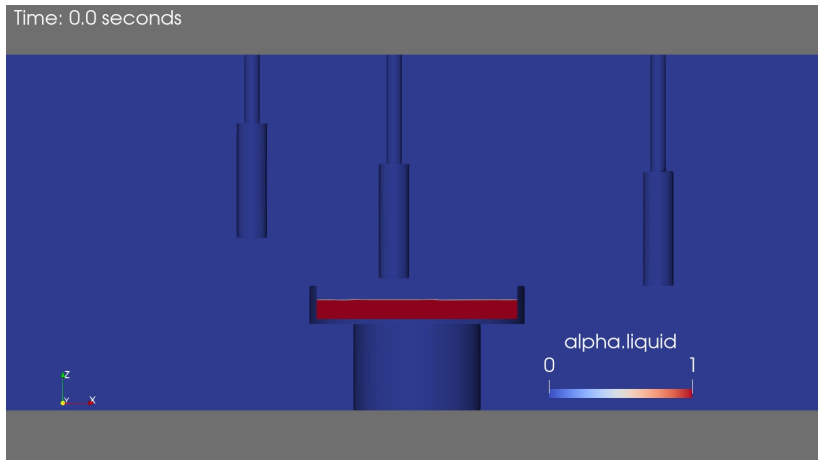


Figure 4.8: FVM simulation result: The initial state of VoF alpha field profile.
The color indicates different types of phase: air phase(blue), and water phase (red). Only the cross section of the 3D domain is shown.
Adopted from [LEE ET AL. 2022c].

humidity case. The relative humidity profile in the computational domain, especially around the free surface region, stays almost the same as if it is a (quasi-) steady state solution. Note that the relative humidity values within the liquid water cells (with α_{water}) are neither used for the calculation nor meaningful.

As it can be assumed from the vapor distribution profile, the evaporation rate or mass reduction rate from the simulation is constant over time once the mass reduction rate is stabilized as in Figure 4.10. Note that at the early time steps, before 1s, the actual mass reduction rate is non-linear since the relative humidity around the free surface has ambient values. Nevertheless, it reaches a linear rate shortly after vapor is diffused from the free surface, and the non-linear behavior is negligible.

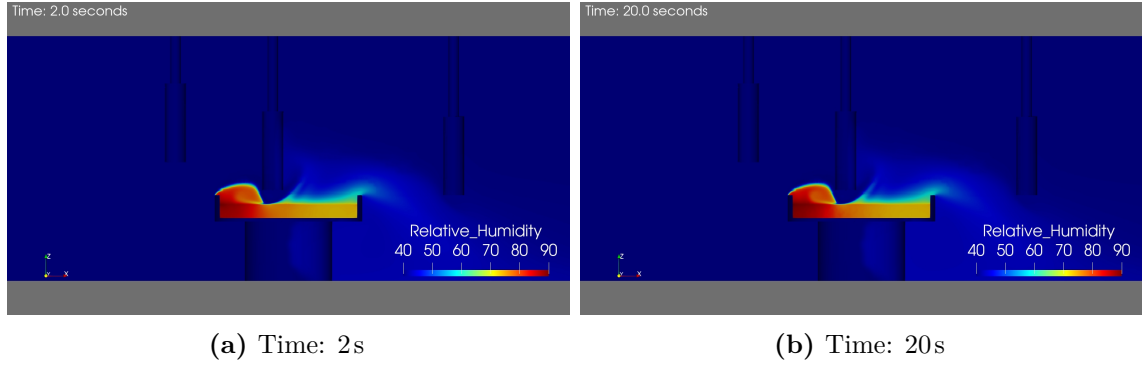


Figure 4.9: FVM simulation result: Virtually constant vapor distribution within the domain over time – resulting in constant evaporation rate. Only the cross section of the 3D domain is shown. Adopted from [LEE ET AL. 2022c].

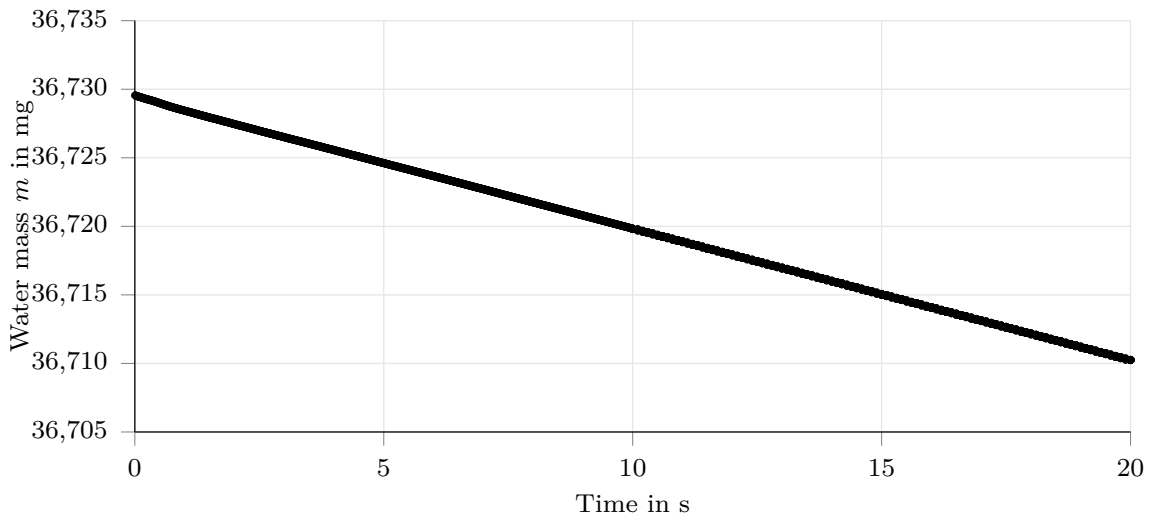


Figure 4.10: FVM multi-phase simulation result: Leftover water mass over time for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 40.6% relative humidity. Adopted from [LEE ET AL. 2022c].

Convergence study

It is never trivial to perform convergence studies or mesh independency studies for the simulation solutions. Since the solution highly depends on the mesh coarseness, especially near the free surface regions, the mesh should be fine enough to keep a sharp phase interface as well as to accurately resolve the vapor concentration gradient. As one example of a mesh independency study, for the sake of brevity, the evaporation rate along the mesh fineness is depicted in Figure 4.11, noting that the condition is $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 40.6% relative humidity case. Here, the evaporation rate converges to approximately $57.7 \frac{\text{mg}}{\text{min}}$ as the mesh becomes finer.

As shown in the convergence study graph in Figure 4.11, the use of $2,780 \times 10^3$ cells for the entire computation domain provides sufficient resolution for validation comparisons

in this specific airflow rate case. The total numbers of cells used for other airflow rate simulation cases are detailed in Table 4.1, located in Section 4.3.

Through these convergence studies, accurate evaporation rates for each boundary condition case can be obtained. The actual numerical results for the validation are compared in the following section.

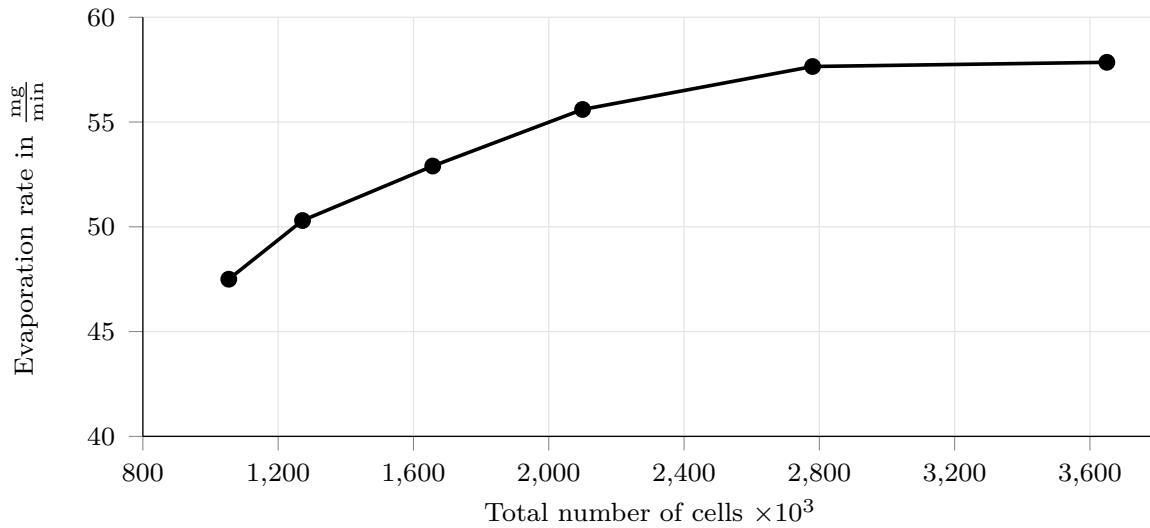


Figure 4.11: Convergence study with respect to the number of cells for the $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 40.6% relative humidity.

Result comparison

A detailed comparison of the results of the experiments with those of the FVM simulations can be found in Figures 4.12a, 4.12b and 4.12c for the three different airflow rates ($1.0 \frac{\text{m}}{\text{s}}$, $1.8 \frac{\text{m}}{\text{s}}$, $2.7 \frac{\text{m}}{\text{s}}$), respectively.

In each figure, the x -axis represents the ambient relative humidity, whereas the y -axis represents the resulting evaporation rate. The blue solid lines and marker points demonstrate the experimental results, and the red dashed lines and marker points show the simulation results. The three ambient air temperatures are represented by different types of marker points – triangular markers for 32.2°C , square markers for 20.5°C , and circular markers for 10.6°C . The equilibrium water body temperature, which is imposed as the initial condition in each simulation, is indicated in brackets near each measurement point. It should also be noted that the specified ambient air temperatures in the experiments are subject to a measurement accuracy of within $\pm 0.5^\circ\text{C}$. The error bars accompanying the experimental measurements are derived from the accuracy of the measurement equipment and the specifications of the climate chamber.

The results of the measurements exhibit that the evaporation rate increases with both higher inlet air temperature and airflow rate, as expected. Additionally, the evaporation rate decreases linearly with increasing relative humidity. The experiments also reveal a quasi-linear relationship between the evaporation rate and airflow rate. The linear slope

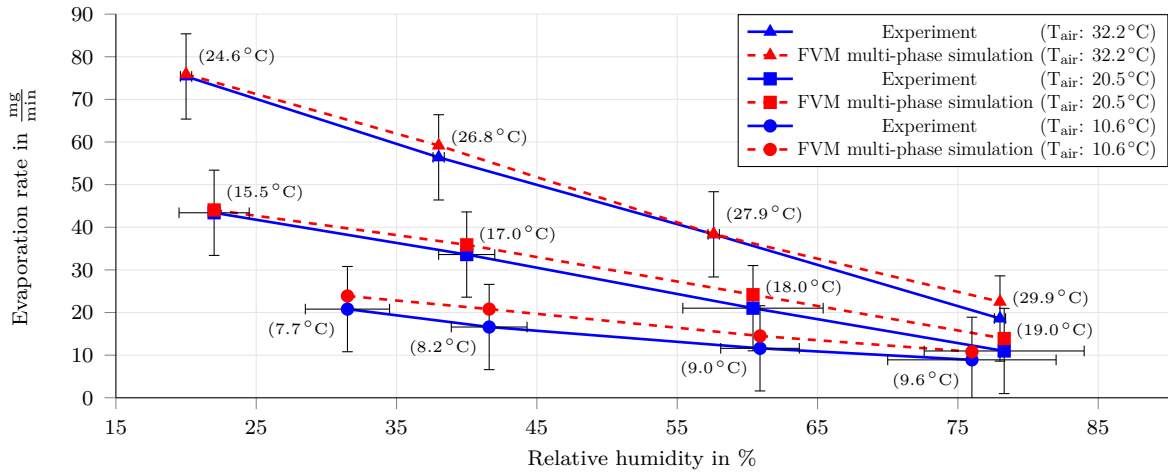
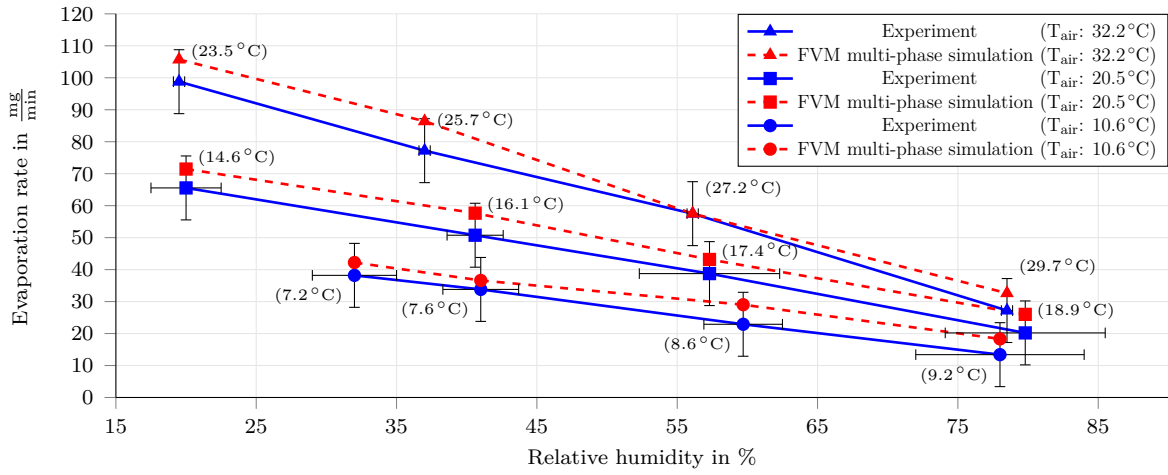
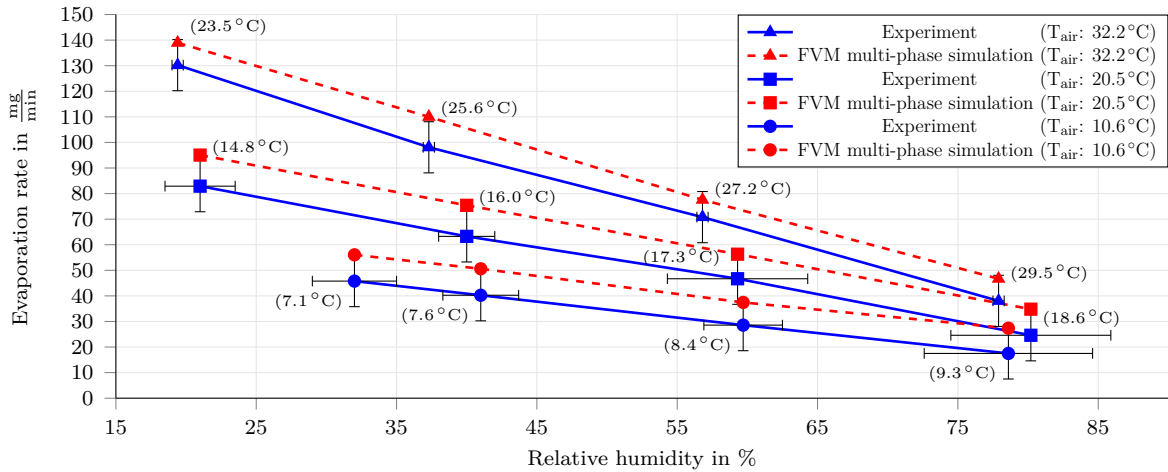
(a) $1.0 \frac{m}{s}$ airflow rate cases(b) $1.8 \frac{m}{s}$ airflow rate cases(c) $2.7 \frac{m}{s}$ airflow rate cases

Figure 4.12: FVM multi-phase simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2022c].

that prevails for higher temperatures (at around 32°C) decreases at lower temperatures. Thus, the effects of the airflow rate are less for lower temperature conditions. Further, the evaporation rate increases exponentially when the ambient air temperature increases. As the saturation vapor pressure of water surges exponentially with temperature, this behavior has also been observed in the literature as well [ÇENGEL & GHAJAR 2014]. Finally, the equilibrium water body temperature is lower when the evaporation rate is higher for all given conditions.

The FVM simulation results closely match the experimental data, falling mostly within the expected margin of measurement error. However, it tends to overestimate evaporation rates, particularly at higher airflow rates. A quantified comparison between simulations and experiments is provided in Section 4.3.

4.2.2 MESHFREE single-phase results

As explained in Section 3.6.2, a constant mass transfer coefficient, as well as constant ambient air temperature/relative humidity values, are imposed for each case of water-only single-phase in GFDM simulations. Thus, identical evaporation rates for all free surface points are observed as depicted in Figure 4.13. In this context, the negative value indicates a mass reduction rate at the free surface. The overall evaporation rate is determined by integrating the local evaporation rate at each point over the entire free surface area.

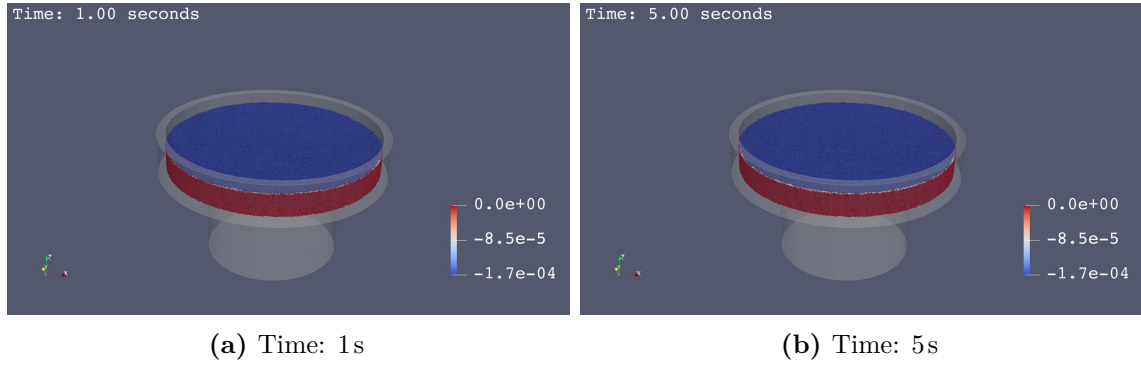


Figure 4.13: Water-only single-phase simulation result: Constant evaporation rate at the free surface points over time indicated by the color scale – identical evaporation rate profile for both 1s and 5s. Adopted from [LEE ET AL. 2023a].

Mass transfer coefficient

In order to correctly simulate the evaporation rate, the averaged mass transfer coefficient $\alpha_{\text{air, mass}}$ using the Sherwood number estimation as described in Section 3.6.2 should be determined. Here, the radius of the water vessel is used as the length scale, i.e., $L = 40\text{ mm}$. Furthermore, a constant value of $Sc = 0.7$ for the Schmidt number [HICKEY ET AL. 2000, ÇENGEL 2002] is assumed. The Reynolds number is obtained as follows according to Equation (3.71): $Re = 2222$ for $1.0 \frac{\text{m}}{\text{s}}$ airflow rate, $Re = 4000$ for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, and $Re = 6000$ for $2.7 \frac{\text{m}}{\text{s}}$ airflow rate. This results in the following mass transfer coefficients:

$$\alpha_{\text{air, mass}} = \begin{cases} 0.106 \frac{\text{m}}{\text{s}} (10.6^\circ\text{C}), 0.113 \frac{\text{m}}{\text{s}} (20.5^\circ\text{C}), 0.120 \frac{\text{m}}{\text{s}} (32.2^\circ\text{C}) \\ \quad \text{for } 1.0 \frac{\text{m}}{\text{s}} \text{ airflow rate,} \\ 0.191 \frac{\text{m}}{\text{s}} (10.6^\circ\text{C}), 0.203 \frac{\text{m}}{\text{s}} (20.5^\circ\text{C}), 0.216 \frac{\text{m}}{\text{s}} (32.2^\circ\text{C}) \\ \quad \text{for } 1.8 \frac{\text{m}}{\text{s}} \text{ airflow rate,} \\ 0.286 \frac{\text{m}}{\text{s}} (10.6^\circ\text{C}), 0.304 \frac{\text{m}}{\text{s}} (20.5^\circ\text{C}), 0.324 \frac{\text{m}}{\text{s}} (32.2^\circ\text{C}) \\ \quad \text{for } 2.7 \frac{\text{m}}{\text{s}} \text{ airflow rate,} \end{cases} \quad (4.1)$$

where the temperatures specified in the brackets correspond to the ambient air temperature. It should also be noted that the calculated mass transfer coefficient depends on the ambient air temperature since the vapor mass diffusivity in air D_{vap} depends on the temperature.

Result comparison

Using the above-calculated mass transfer coefficient values, a detailed comparison of the results of the experiments with those of the single-phase simulations can be found in Figures 4.14a, 4.14b and 4.14c. The structure of the graph is previously stated in Section 4.2.1. Note that a convergence study is not necessary for the single-phase GFDM approach since the evaporation rate is resolved by user-calculated coefficient and boundary conditions at each free surface point globally. Thus, it should be sufficient for the simulation to have the point cloud which is fine enough only to cover the free surface region without any significant deformation. Any further refinement has minimal effects on the simulated evaporation rate.

The single-phase numerical results show a close correlation with the experimental ones. However, the evaporation rate is overestimated for higher temperatures with lower relative humidity. Additionally, for higher temperature cases, the simulation shows that the evaporation rate decreases more steeply with increasing controlled relative humidity compared to the experimental results. This discrepancy highlights a fundamental limitation of the single-phase approach: its inability to accurately capture the airflow dynamics around the phase interface and the absence of a universal mass transfer coefficient.

4.2.3 MESHFREE multi-phase results

In this section, the numerical results of GFDM multi-phase approaches for both coupling schemes – surface-surface-coupling and volume-volume-coupling – are shown. First, the relative humidity profile of numerical simulation over time with the corresponding geometry and with the initial water reservoir is shown in Figure 4.15. Here, the water phase points always show the saturated vapor concentration, or 100% relative humidity, noting that the point cloud is only refined around the user-pre-defined free surface, water vessel, and humidity/temperature sensor regions in order to correctly resolve the evaporation physics at the water-air interface as well as turbulent effects in the air [LEE ET AL. 2023a]. From the results, it is observed that the generated vapor from the water surface is well diffused from the higher-concentrated to the lower-concentrated regions and also convected by the forced airflow from channel inlet to outlet.

Quasi-steady state evaporation rate

As shown from Figure 4.15, the vapor profile does not change drastically over time, but overall picture is relatively stable, especially near the free surface. Hence, the

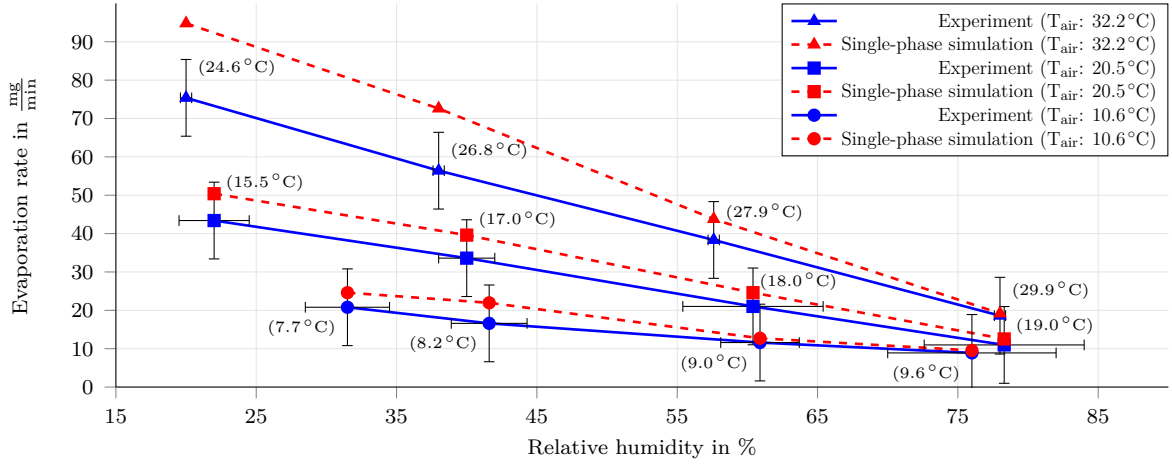
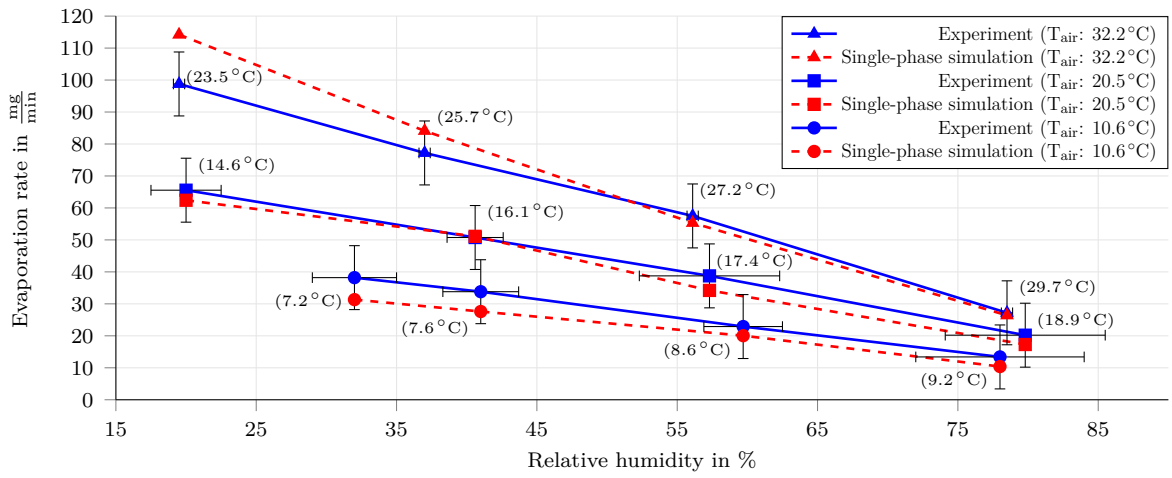
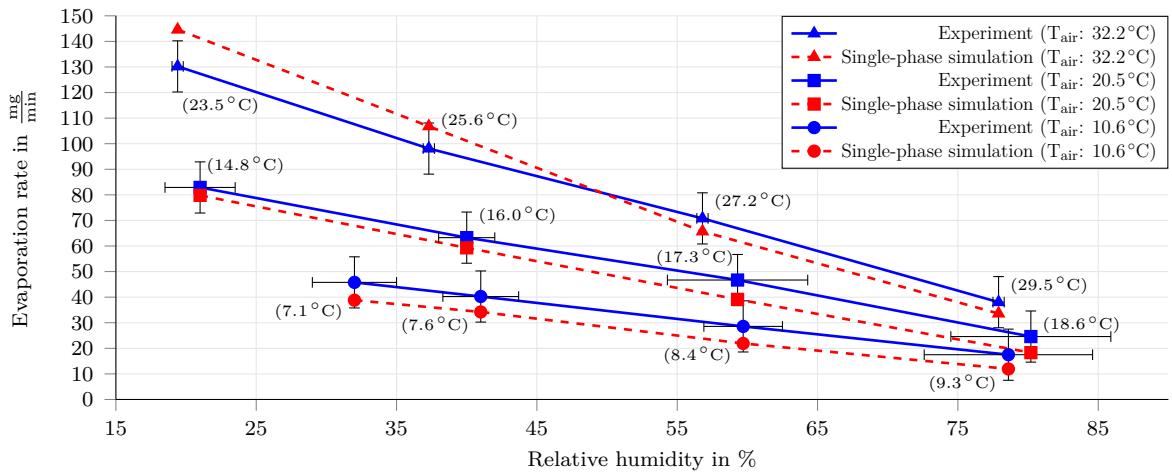
(a) 1.0 $\frac{\text{m}}{\text{s}}$ airflow rate cases(b) 1.8 $\frac{\text{m}}{\text{s}}$ airflow rate cases(c) 2.7 $\frac{\text{m}}{\text{s}}$ airflow rate cases

Figure 4.14: Single-phase simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2023a].

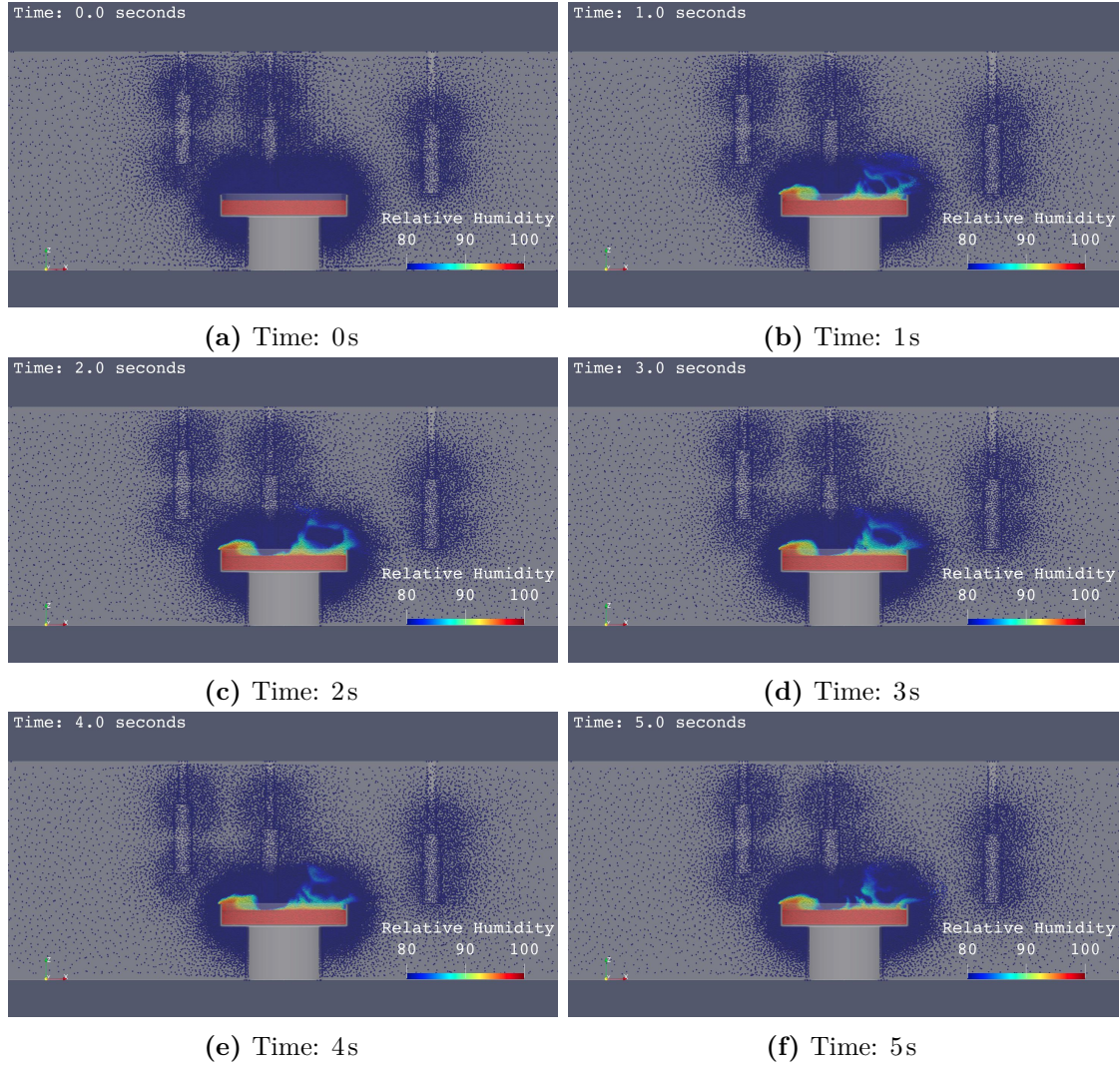


Figure 4.15: Multi-phase simulation result with pre-defined regional refinement: Relative humidity profile from 0s to 5s in the cross section of the domain for $1.0 \frac{\text{m}}{\text{s}}$ airflow rate, 32.2°C air temperature, and 78% relative humidity. Adopted from [LEE ET AL. 2023a].

numerical evaporation rate can be determined by integrating the calculated mass flux $\left(\frac{\text{kg}}{\text{m}^2 \cdot \text{s}}\right)$ over the entire interface with respect to the associated area of the interface points. The calculated evaporation rate over time is depicted in Figure 4.16. Similar to the FVM simulation cases, the evaporation rate reaches a quasi-steady value of $14 \frac{\text{mg}}{\text{min}}$ approximately after 0.7s, even though it shows small fluctuations ($\pm 5\%$ around the mean value), which is presumably due to the Lagrangian nature of the simulation [LEE ET AL. 2023a]. It should be noted that finer point clouds reduce the fluctuations and also lead to a quasi-steady state. Details regarding mean evaporation rate convergence with respect to the point cloud resolution is described in Figure 4.19 in this section.

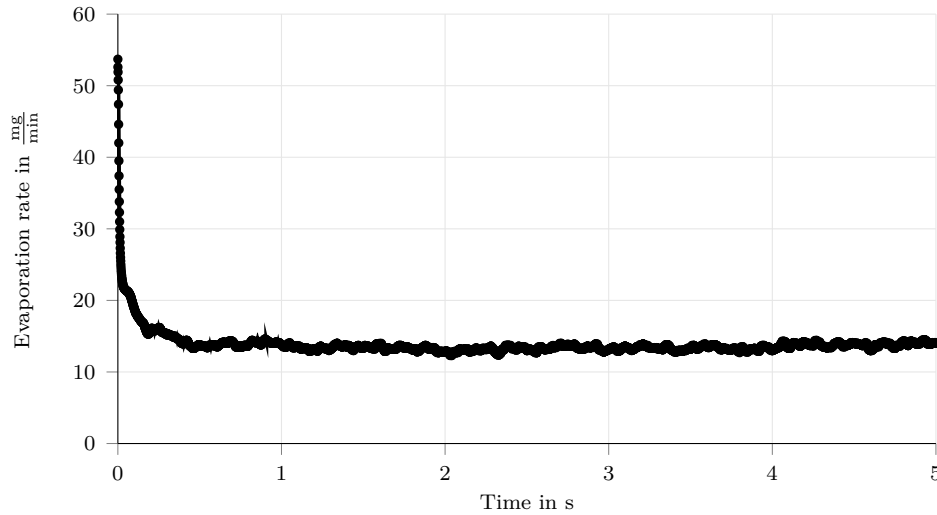


Figure 4.16: Multi-phase simulation result with pre-defined regional refinement: Evaporation rate over time for $1.0 \frac{\text{m}}{\text{s}}$ airflow rate, 32.2°C air temperature, and 78% relative humidity. Adopted from [LEE ET AL. 2023a].

Automatic adaptive refinement

One of the most advantageous characteristics of the meshfree GFDM over traditional mesh-based methods is the capability of deploying an adaptive refinement of the point cloud. This feature performs refinement during the simulation runtime based on user-defined criteria, which is nearly computationally free. On the contrary, in mesh-based methods, deploying runtime adaptive refinement can be inefficient due to the generally time-consuming and computationally expensive nature of the meshing-and-remeshing process, especially when dealing with complex geometries. By introducing an adaptive refinement feature based on the local vapor concentration gradient and velocity gradients, as well as free surface region, the computation time in the GFDM can be significantly reduced. Additionally, this automated adaptive refinement feature eliminates the need for manual local refinement definitions, simplifying the extension of the developed evaporation simulation method to arbitrary and more intricate geometries [LEE ET AL. 2022b].

The adaptive refinement simulation results with humidity profile over time for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.2°C air temperature, and 57.3% relative humidity case are shown in Figure 4.17. At the initial state, the point cloud around the water phase and free surface is dense, whereas the air phase has a coarse point cloud in the entire domain. As the simulation advances, it autonomously identifies areas with high humidity- and velocity gradients, subsequently refining the point cloud accordingly. This automated process ensures the accurate capturing of gradients around the phase interface and the geometries of the vessel/sensor. Another adaptive optimization point arises from the observation that the simulation requires some time to attain a quasi-steady state evaporation rate. For example, as shown in Figure 4.16, it takes approximately 0.7s simulation time to reach the quasi-steady state. Therefore, extensive refinement during

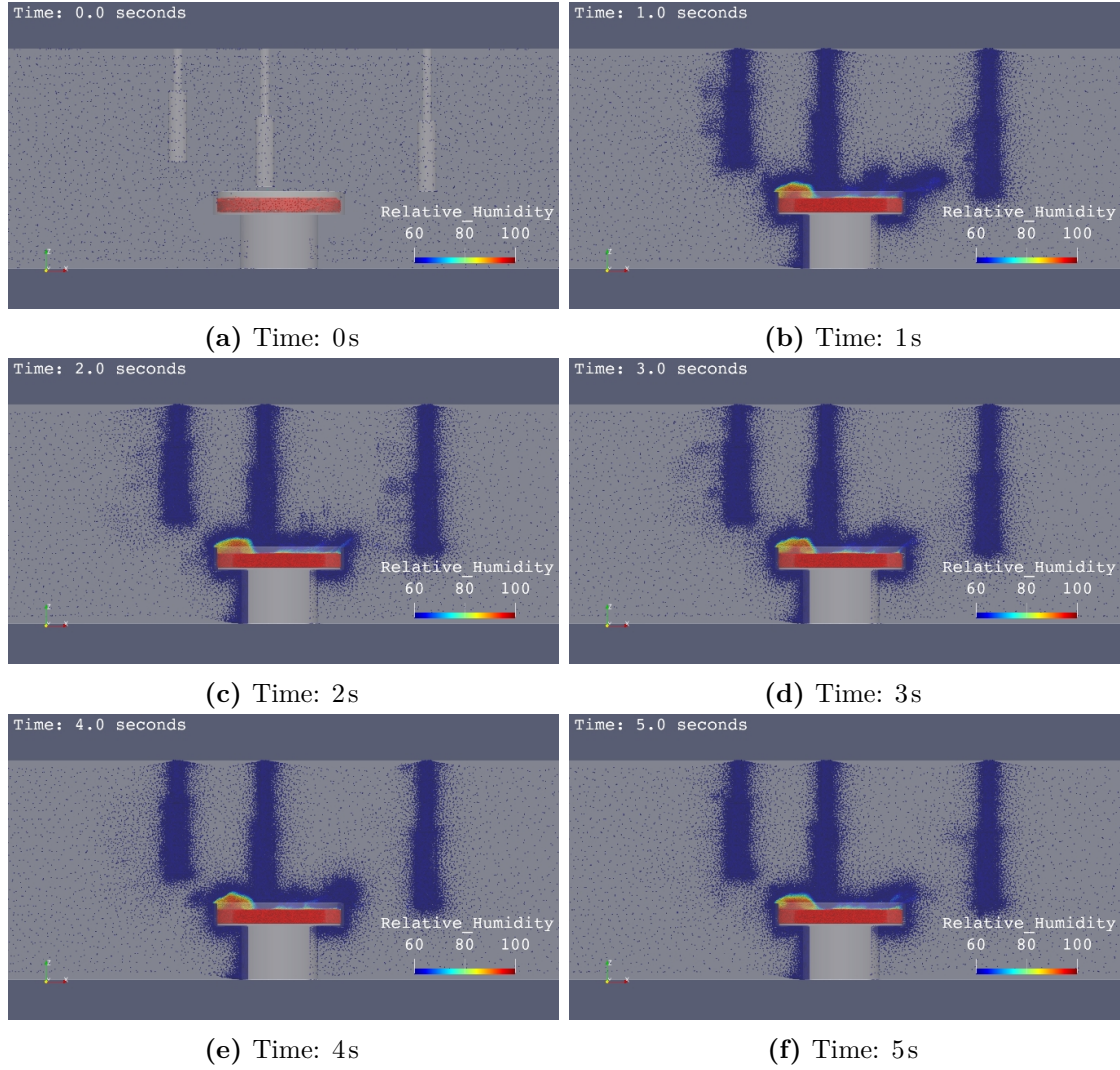


Figure 4.17: Multi-phase simulation result with adaptive refinement refinement: Relative humidity profile from 0s to 5s in the cross section of the domain for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 57.3% relative humidity. Adapted from [LEE ET AL. 2022b].

the initial stages of the simulation is unnecessary. Exploiting this can lead to a reduction in runtime overheads. This time frame is denoted as “startup time”.

The resulting evaporation rate over time with the deployment of autonomous adaptive refinement for both with and without startup time is depicted in Figure 4.18. Similar to the manual regional refinement cases, the calculated evaporation rate reaches a quasi-steady state value after some simulation time, say approximately 0.7–1.0s, noting that the evaporation rate exhibits distinct behavior in the early time steps due to different point cloud resolutions during this time frame. According to the research, speedup ratios of approximately 1.36 (without startup time) and 1.57 (with startup time) are obtained when the adaptive refinement is deployed, noting that it can have slight variations depending on the conditions such as atmospheric boundary conditions and number of cores used. Moreover, the resulting quasi-steady state evaporation rate

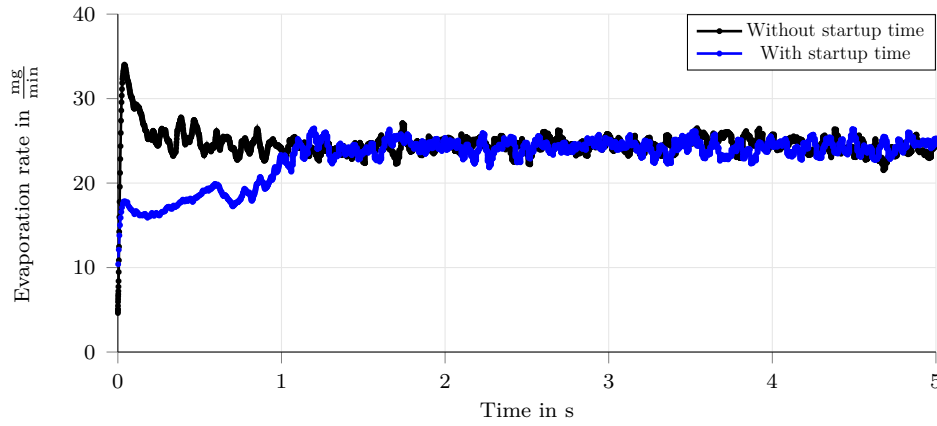


Figure 4.18: Multi-phase simulation result with adaptive refinement with (black) and without (blue) startup time: Evaporation rate over time for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.2°C air temperature, and 57.3% relative humidity. Adopted from [LEE ET AL. 2022b].

with adaptive refinement is slightly lower (approximately 13%) than that of the manual local refinement cases, which may arise not thoroughly resolved gradients. [LEE ET AL. 2022b] In conclusion, utilizing automated adaptive refinement makes the method faster in runtime and gives further flexibility to be deployed in any arbitrary geometries only with minimal effects on the accuracy.

Convergence study

Analogous to the mesh-based FVM solver demonstrated in Section 4.2.1, a convergence study is conducted for each simulation case to determine the necessary point cloud resolution and the number of points. Figure 4.19 depicts the convergence study results of the $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 57.3% relative humidity case, as one example of such convergence study in MESHFREE.

The evaporation rate to be used for validation can be obtained through the convergence study for each case, like in the FVM cases, which will be presented in the following sections.

Surface-surface-coupling approach result comparison

A detailed comparison of the validation results with the surface-surface coupling approach is presented in Figure 4.20a, 4.20b and 4.20c for the three different airflow rates ($1.0 \frac{\text{m}}{\text{s}}$, $1.8 \frac{\text{m}}{\text{s}}$, $2.7 \frac{\text{m}}{\text{s}}$). The general format of the figures is explained in Section 4.2.1. It should also be noted that the results for the surface-surface-coupling approach are without the application of the adaptive refinement feature for the data consistency with the publication LEE ET AL. 2023, which is published before the full implementation of this feature.

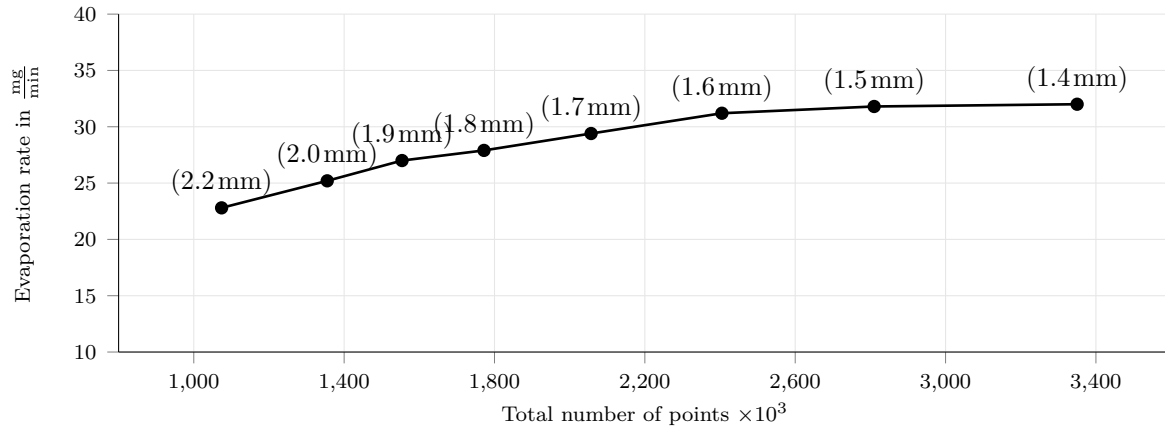


Figure 4.19: Convergence study with respect to the point cloud resolution for the $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 57.3% relative humidity. The bracketed values next to the marker points indicate the minimum point cloud resolution around the water-air interface. Adopted from [LEE ET AL. 2023a].

The simulation results exhibit a good agreement with the experimental data within the anticipated margin of measurement errors. Furthermore, the trend line with respect to ambient relative humidity aligns well with that of the corresponding experiment across all temperatures. In Section 4.3, a quantitative comparison between simulations and experiments is presented.

Volume-volume-coupling approach result comparison

For the volume-volume-coupling cases, the full feature of the time- and location-dependent adaptive refinement is deployed [LEE ET AL. 2022b, LEE ET AL. 2024]. The general pattern of the humidity profile is practically the same as Figure 4.17. Moreover, the evaporation rate reaches a quasi-steady state value as depicted with the startup graph in Figure 4.18. The validation results of the volume-volume-coupling are described in Figure 4.21a, 4.21b and 4.21c as previous comparisons. The simulation outcomes exhibit a strong correlation with the experimental measurements, as well shown in the figures. A quantitative comparison will be followed in the next section.

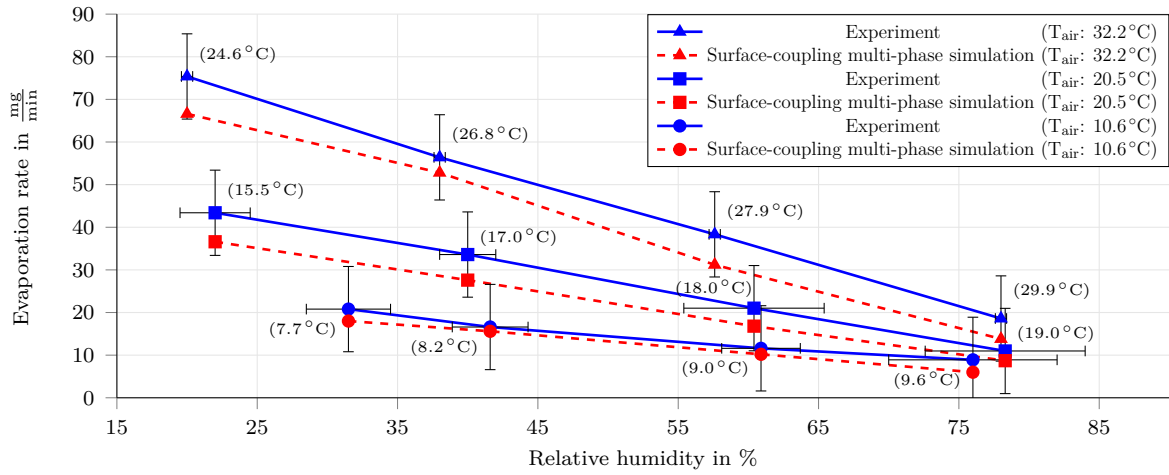
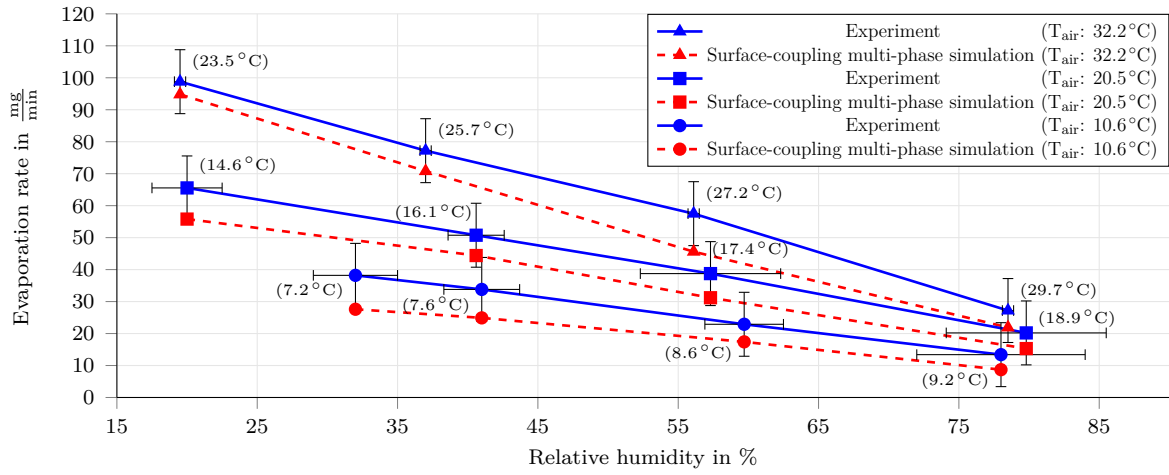
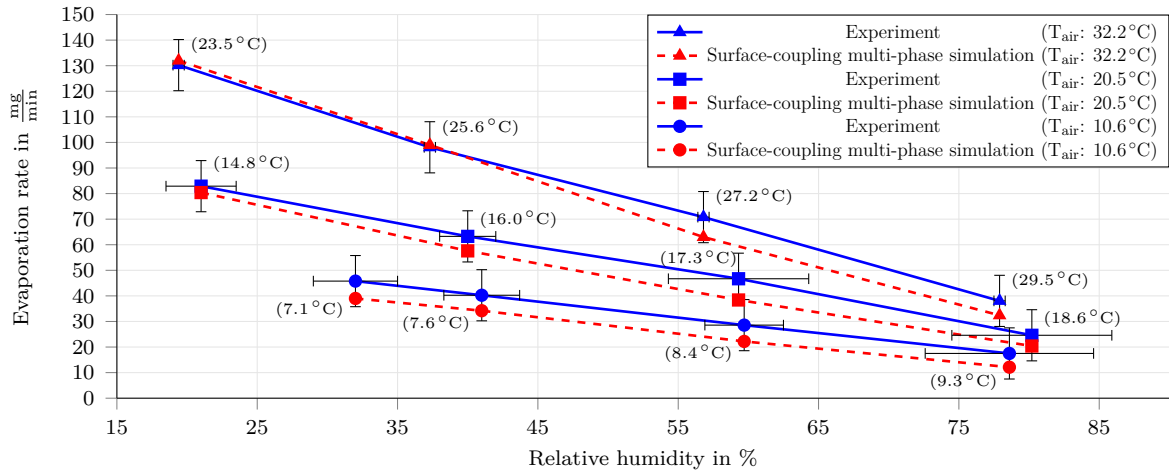
(a) 1.0 $\frac{m}{s}$ airflow rate cases(b) 1.8 $\frac{m}{s}$ airflow rate cases(c) 2.7 $\frac{m}{s}$ airflow rate cases

Figure 4.20: Surface-surface-coupling simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2023a].

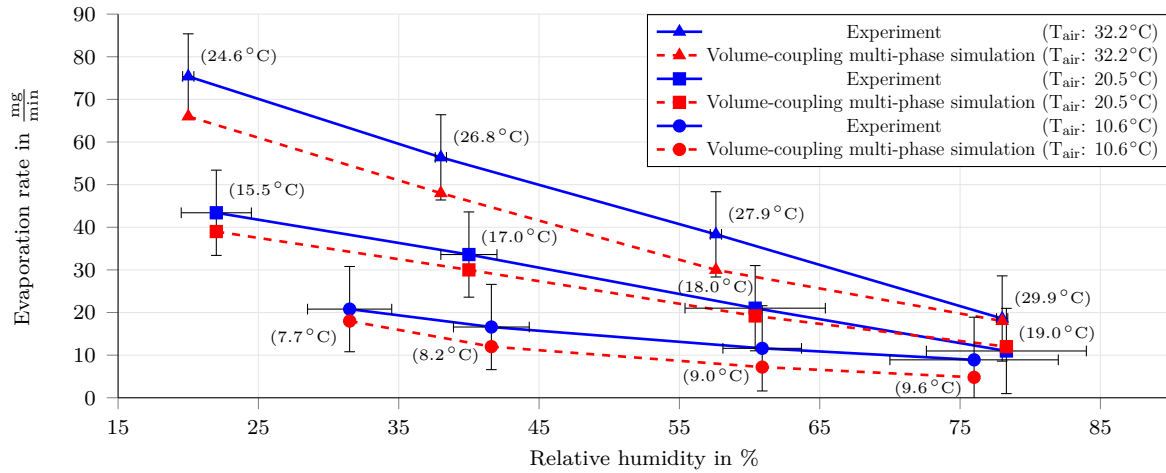
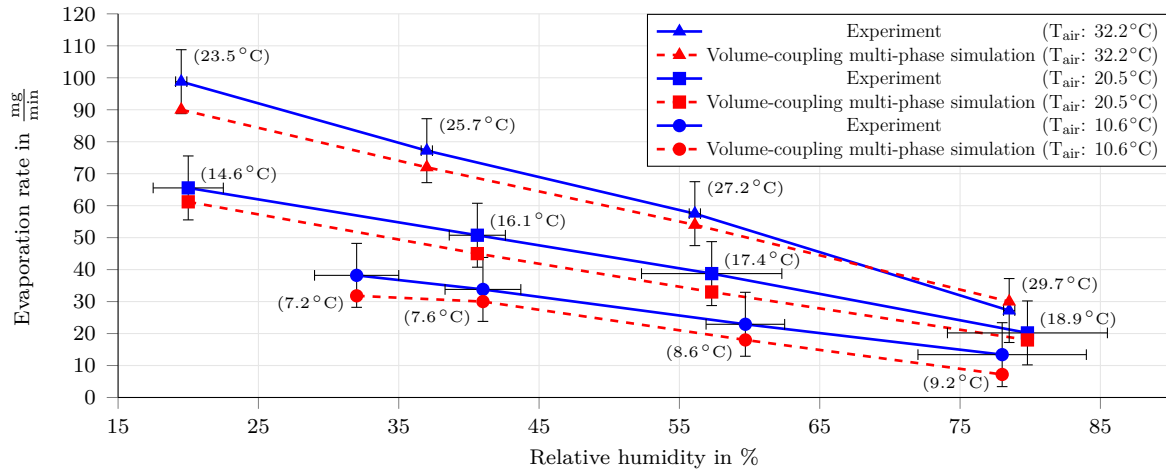
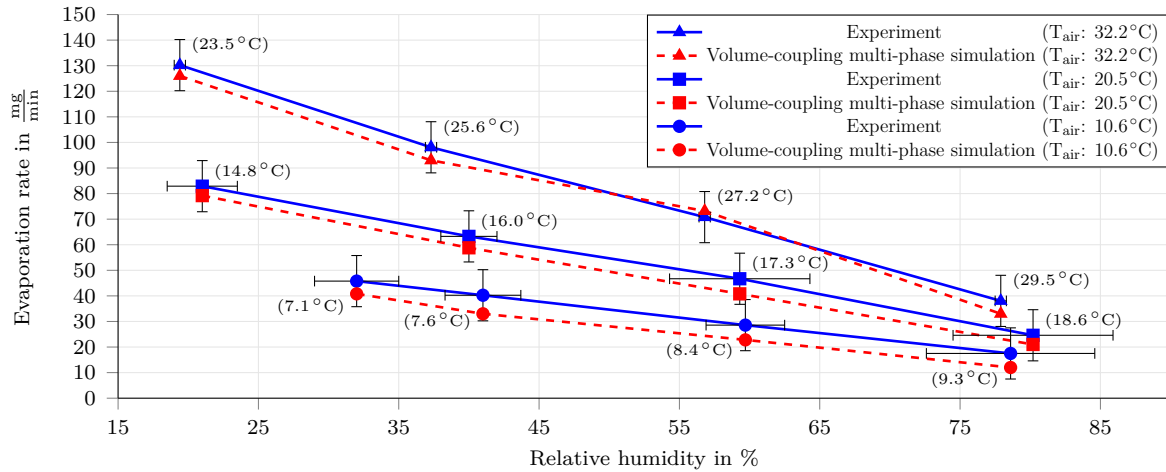
(a) 1.0 $\frac{\text{m}}{\text{s}}$ airflow rate cases(b) 1.8 $\frac{\text{m}}{\text{s}}$ airflow rate cases(c) 2.7 $\frac{\text{m}}{\text{s}}$ airflow rate cases

Figure 4.21: Volume-volume-coupling simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2024].

4.3 Validation results comparison and discussion

The validation results are compared and discussed in various points. Based on the comparisons, a discussion regarding which approach is more suitable for further application is also stated at the end.

4.3.1 Runtime Comparison

First of all, the runtime comparison of each approach is presented in Table 4.1. Note that all simulation executions were conducted using identical hardware configurations with the same number of cores. This was done primarily to assess the relative differences in runtime. In this context, the runtime refers to the total clock time for the entire simulation. For the FVM cases, the time for the pre-processing, such as the meshing process, which usually takes less than an hour in the parallel run, is also included. In GFDM approaches, this covers the reading of the bounding geometry, initialization, and management of the point clouds, as well as post-processing to determine mass fluxes and evaporation rates.

The runtime comparison is only made with respect to the three airflow rates as the runtime depends highly on the airflow rate, while only negligible effects due to changes in atmospheric air temperature and humidity are observed. Therefore, other atmospheric conditions for the simulation runs in the runtime comparison are identical such that 20.5 °C and roughly 60 % humidity.

For multi-phase approaches, either with the GFDM or the FVM, the simulations run longer when the airflow rate increases for two reasons: a) Due to the CFL conditions (or CFL-like restrictions in Lagrangian movement [SUCHDE & KUHNERT 2018]), larger airflow velocities result in lower time step sizes. b) A larger number of discretization elements (cells or points) is required to accurately resolve the flow physics and concentration gradients at the interface.

In contrast, for the GFDM single-phase approach, the required point cloud resolution barely depends on the airflow rate. It is sufficient if the point cloud is dense enough to resolve the free surface region correctly in general. Nevertheless, the same point cloud resolutions on the water side for both approaches are used for the same airflow rates. Note that the total number of points shown in Table 4.1 includes both air and water phase points for the multi-simulations, which makes a significant difference compared to that of the single-phase.

The runtime comparison shows that the multi-phase simulations are much more computationally intensive (factor of 20-50), which is expected. In general, the FVM multi-phase approach shows shorter runtime compared to the GFDM multi-phase approaches since, in GFDM, it requires time to search and redefine the neighbor point for stencil generation in each time step. Within the GFDM multi-phase approaches, the automatic adaptive refinement is used for the volume-volume-coupling, whereas the original regional refinement is deployed for the sake of consistency with the publications

Table 4.1: Runtime comparison for 5s of simulation time for different airflow rates, 20.5°C air temperature, and approximately 60% relative humidity. Partly adapted from [LEE ET AL. 2023a].

Type	# of points or cells	# of cores	Runtime
Airflow rate: $1.0 \frac{\text{m}}{\text{s}}$			
FVM Multi-phase simulation	$2,378 \times 10^3$	240	39.6h
Single-phase simulation	378×10^3	240	2.28h
Surface-coupling Multi-phase simulation (regional refinement)	$2,000 \times 10^3$	240	52.81h
Volume-coupling Multi-phase simulation (adaptive refinement)	$2,020 \times 10^3$	240	53.81h
Airflow rate: $1.8 \frac{\text{m}}{\text{s}}$			
FVM Multi-phase simulation	$2,780 \times 10^3$	240	62.26h
Single-phase simulation	444×10^3	240	2.83h
Surface-coupling Multi-phase simulation (regional refinement)	$2,405 \times 10^3$	240	98.24h
Volume-coupling Multi-phase simulation (adaptive refinement)	$2,400 \times 10^3$	240	96.81h
Airflow rate: $2.7 \frac{\text{m}}{\text{s}}$			
FVM Multi-phase simulation	$3,120 \times 10^3$	240	104.28h
Single-phase simulation	550×10^3	240	3.83h
Surface-coupling Multi-phase simulation (regional refinement)	$2,810 \times 10^3$	240	150.33h
Volume-coupling Multi-phase simulation (adaptive refinement)	$2,650 \times 10^3$	240	146.81h

([LEE ET AL. 2023a] and [LEE ET AL. 2024]). Originally, the volume-volume-coupling approach should have at least as many more points as single-phase than the surface-surface-coupling since the air points overlap the water phase. However, due to the adaptive refinement feature, it has nearly the same number of points or sometimes even less compared to the surface-surface-coupling. Consequently, the runtime difference between the GFDM multi-phase approaches is not significant.

4.3.2 Error Comparison

The relative deviations of the numerical evaporation rates from the experimental ones are summarized in Table 4.2, 4.3 and 4.4. Here, the measurement uncertainties in the experiments are also appended for a better overview of the numerical results. In this context, the positive sign represents a higher evaporation rate compared to the

corresponding measurement, and the negative sign represents a lower evaporation rate.

Also, note that the highlighted values mean the simulation result is out of the measurement uncertainty range. Higher relative errors are observed for high relative humidity as well as low-temperature cases. This is because of the fact that the absolute evaporation rates are relatively small, and even a minor absolute deviation can result in a substantial relative error.

Additionally, the ambient relative humidity inside the climate chamber has more significant fluctuations in the experiments in these cases, as maintaining stable conditions proves challenging for the chamber regulator. This eventually leads to larger errors in the measurements.

There are some cases that the simulation outcomes are out of range of the measurement uncertainties, especially with the FVM and GFDM single-phase approaches. Nevertheless, overall, the validation of the newly developed methods with different approaches for evaporation shows good correlation to the experimental results within the measurement uncertainties.

4.3.3 Overall discussion of various approaches

The evaporation rates predicted by FVM are generally higher than the actual experimental results. This discrepancy can be attributed to several factors, particularly the potential overestimation of the turbulence model, which may inaccurately predict the mixing behavior around the free surface. This issue is especially pronounced in scenarios with high airflow rates, resulting in enhanced evaporation rates that do not fully align with the observed data. Additionally, numerical diffusion inherent in the FVM approach can smooth out sharp gradients, further contributing to these overestimations of evaporation fluxes.

Despite these challenges, it is noteworthy that the FVM outcomes demonstrate a strong correlation with the experimental results, remaining within the expected error margins and closely following the overall trend.

Although the FVM solution is successfully validated, it does have some restrictions. For instance, meshing and remeshing may be required during simulation runtime to maintain sharp interface regions and accurately calculate humidity gradients. Additionally, defining regional refinements of the initial status for each geometry formation must be done manually by the user.

Given the ultimate goal of constructing an automated simulation pipeline for water evaporation in complex vehicle geometries without manual geometry clean-up procedures, GFDM approaches are more suitable for practical applications.

The GFDM single-phase approach is very efficient in terms of computation time and simplicity [LEE ET AL. 2023a]. However, unlike the water vessel geometry or any other geometric formations, where semi-empirical mass transfer coefficients can be

Table 4.2: Comparison of simulations and experiments: Relative error of the numerical evaporation rates with respect to the experimental data for the $1.0 \frac{\text{m}}{\text{s}}$ airflow rate. The highlighted values indicate that the simulation error is larger than the measurement uncertainty. Partly adapted from [LEE ET AL. 2023a].

Airflow rate: $1.0 \frac{\text{m}}{\text{s}}$		Air temperature: 32.2°C			
Type \ Humidity		20.0 %	38.0 %	57.6 %	78.0 %
FVM Multi-phase simulation		0.68 %	4.92 %	0.13 %	21.13 %
Single-phase simulation		25.76 %	27.66 %	14.24 %	3.22 %
Surface-coupling Multi-phase simulation (regional refinement)		-11.65 %	-6.38 %	-18.62 %	-25.81 %
Volume-coupling Multi-phase simulation (adaptive refinement)		-12.44 %	-14.89 %	-21.75 %	-3.22 %
Measurement uncertainty		$\pm 13.27 \%$	$\pm 17.73 \%$	$\pm 26.08 \%$	$\pm 53.76 \%$
		Air temperature: 20.5°C			
Type \ Humidity		22.0 %	40.0 %	60.4 %	78.3 %
FVM Multi-phase simulation		1.52 %	6.78 %	15.04 %	26.60 %
Single-phase simulation		16.13 %	17.86 %	17.03 %	14.20 %
Surface-coupling Multi-phase simulation (regional refinement)		-15.67 %	-17.86 %	-20.08 %	-20.77 %
Volume-coupling Multi-phase simulation (adaptive refinement)		-10.13 %	-10.71 %	-8.66 %	-9.29 %
Measurement uncertainty		$\pm 23.04 \%$	$\pm 29.76 \%$	$\pm 47.57 \%$	$\pm 91.07 \%$
		Air temperature: 10.6°C			
Type \ Humidity		31.5 %	41.6 %	60.9 %	76.0 %
FVM Multi-phase simulation		14.83 %	25.30 %	25.01 %	21.34 %
Single-phase simulation		18.26 %	32.28 %	9.66 %	7.19 %
Surface-coupling Multi-phase simulation (regional refinement)		-13.46 %	-6.02 %	-12.07 %	-32.58 %
Volume-coupling Multi-phase simulation (adaptive refinement)		-13.46 %	-27.71 %	-37.93 %	-46.06 %
Measurement uncertainty		$\pm 48.08 \%$	$\pm 60.24 \%$	$\pm 86.21 \%$	$\pm 112.35 \%$

applicable [ÇENGEL & GHAJAR 2014], it is usually troublesome to correctly obtain a mass transfer coefficient and the corresponding averaged convective mass transfer value when the geometry becomes complex. Even for this relatively simple geometry, the semi-empirical mass transfer coefficient may not be fully applicable, which is evident in

Table 4.3: Comparison of simulations and experiments: Relative error of the numerical evaporation rates with respect to the experimental data for the $1.8 \frac{\text{m}}{\text{s}}$ airflow rate. The highlighted values indicate that the simulation error is larger than the measurement uncertainty. Partly adapted from [LEE ET AL. 2023a].

Airflow rate: $1.8 \frac{\text{m}}{\text{s}}$		Air temperature: 32.2°C			
Type	Humidity	19.5 %	37.0 %	56.1 %	78.5 %
FVM Multi-phase simulation		7.02 %	11.91 %	0.15 %	19.98 %
Single-phase simulation		15.41 %	14.25 %	−3.79 %	−2.94 %
Surface-coupling Multi-phase simulation (regional refinement)		−4.03 %	−8.29 %	−20.70 %	−19.49 %
Volume-coupling Multi-phase simulation (adaptive refinement)		−8.88 %	−6.73 %	−6.08 %	−10.29 %
Measurement uncertainty		$\pm 10.12 \%$	$\pm 12.95 \%$	$\pm 17.39 \%$	$\pm 36.76 \%$
		Air temperature: 20.5°C			
Type	Humidity	20.0 %	40.6 %	57.3 %	79.8 %
FVM Multi-phase simulation		9.00 %	13.60 %	11.40 %	28.71 %
Single-phase simulation		−4.81 %	0.72 %	−11.74 %	−14.45 %
Surface-coupling Multi-phase simulation (regional refinement)		−14.87 %	−12.51 %	−19.48 %	−24.26 %
Volume-coupling Multi-phase simulation (adaptive refinement)		−6.63 %	−11.33 %	−14.83 %	−10.89 %
Measurement uncertainty		$\pm 15.25 \%$	$\pm 19.70 \%$	$\pm 25.80 \%$	$\pm 49.50 \%$
		Air temperature: 10.6°C			
Type	Humidity	32.0 %	41.0 %	59.7 %	78.0 %
FVM Multi-phase simulation		10.52 %	8.33 %	26.72 %	36.74 %
Single-phase simulation		−18.01 %	−19.94 %	−12.48 %	−22.40 %
Surface-coupling Multi-phase simulation (regional refinement)		−27.74 %	−26.33 %	−24.02 %	−35.07 %
Volume-coupling Multi-phase simulation (adaptive refinement)		−16.75 %	−11.24 %	−21.38 %	−46.26 %
Measurement uncertainty		$\pm 26.17 \%$	$\pm 29.58 \%$	$\pm 43.66 \%$	$\pm 74.62 \%$

the discrepancies observed in the evaporation rate results. As a result, it is difficult to ascertain whether the predicted values align with the trends of the actual experimental results.

Table 4.4: Comparison of simulations and experiments: Relative error of the numerical evaporation rates with respect to the experimental data for the $2.7 \frac{\text{m}}{\text{s}}$ airflow rate. The highlighted values indicate that the simulation error is larger than the measurement uncertainty. Partly adapted from [LEE ET AL. 2023a].

Airflow rate: $2.7 \frac{\text{m}}{\text{s}}$		Air temperature: 32.2°C			
Type	Humidity	19.4 %	37.3 %	56.8 %	77.9 %
FVM Multi-phase simulation		6.70 %	12.13 %	9.57 %	22.74 %
Single-phase simulation		10.58 %	8.86 %	-7.20 %	-11.68 %
Surface-coupling Multi-phase simulation (regional refinement)		1.37 %	0.92 %	-11.02 %	-14.84 %
Volume-coupling Multi-phase simulation (adaptive refinement)		-3.24 %	-5.19 %	3.39 %	-13.26 %
Measurement uncertainty		$\pm 7.67 \%$	$\pm 10.19 \%$	$\pm 14.12 \%$	$\pm 26.28 \%$
		Air temperature: 20.5°C			
Type	Humidity	21.0 %	40.0 %	59.3 %	80.2 %
FVM Multi-phase simulation		14.65 %	19.18 %	20.55 %	41.46 %
Single-phase simulation		-3.74 %	-6.30 %	-16.23 %	-25.53 %
Surface-coupling Multi-phase simulation (regional refinement)		-3.01 %	-8.96 %	-17.77 %	-17.07 %
Volume-coupling Multi-phase simulation (adaptive refinement)		-4.46 %	-7.06 %	-12.63 %	-14.63 %
Measurement uncertainty		$\pm 12.06 \%$	$\pm 15.80 \%$	$\pm 21.41 \%$	$\pm 40.65 \%$
		Air temperature: 10.6°C			
Type	Humidity	32.0 %	41.0 %	59.7 %	78.6 %
FVM Multi-phase simulation		22.45 %	25.71 %	31.08 %	56.34 %
Single-phase simulation		-15.20 %	-15.03 %	-23.35 %	-31.77 %
Surface-coupling Multi-phase simulation (regional refinement)		-14.81 %	-15.03 %	-22.29 %	-30.74 %
Volume-coupling Multi-phase simulation (adaptive refinement)		-10.87 %	-18.01 %	-20.19 %	-31.42 %
Measurement uncertainty		$\pm 21.84 \%$	$\pm 24.84 \%$	$\pm 35.00 \%$	$\pm 57.14 \%$

The GFDM multi-phase approaches demonstrate strong validation of evaporation rates; however, the predicted rates are generally lower than those observed in experiments. This discrepancy may arise from several factors, including model simplifications and the inadequate consideration of complex phase interactions and dynamics.

In the surface-surface coupling approach, phase coupling conditions can occasionally become unstable in complex geometries. This instability leads to a loss of associated interface points between phases, resulting in breaks in phase coupling and ultimately yielding inaccurate evaporation rates [LEE ET AL. 2024]. Conversely, the volume-volume coupling approach maintains stable phase coupling even when applied to actual complex vehicle geometries with intricate free surface formations.

Given these findings, the GFDM multi-phase method utilizing the volume-volume coupling approach is employed for further investigations.

5 Validation and application to vehicle geometries

The chosen developed method – GFDM MESHFREE multi-phase with the volume-volume-coupling – is applied for further investigations. It is applied to actual vehicle geometries and for dry-out time validations. An experiment series to measure the total dry-out times of an accumulated water source at the corner of the sunroof channel of a vehicle in different ambient conditions is designed for validation. Simulations under identical conditions are conducted. Hereby, in order to extend the time scale of simulations – generally in the order of seconds – to the real-world dry-out time scale – commonly in the order of hours or, days or even weeks – the evaporation rate at the free surface is artificially accelerated to approximate the actual total dry-out time.

5.1 Sunroof channel geometry case for Vehicle A

(The majority of the contents in this section is already published in a journal [LEE ET AL. 2024].)

A thorough dry-out time validation process utilizing the developed numerical approach in the sunroof channel of Vehicle A, including the experimental setup, is demonstrated in this section.

5.1.1 Experiment setup

The complete dry-out time of a water accumulation at the corner of the first vehicle's sunroof channel is assessed under various ambient conditions, which are controlled in a climate chamber. A tiny humidity sensor sized by $10.2\text{mm} \times 5.1\text{mm} \times 1.8\text{mm}$ is positioned precisely at the corner of the sunroof channel to monitor the progression of relative humidity values over time, as depicted in Figure 5.1.

Moreover, to visually examine the development of the drying-out process, snapshot photos are captured at defined time intervals using an endoscope. Simultaneously, at the opposite corner, the body temperature of the water accumulation is measured using a thermometer, as illustrated in Figure 5.2, so as not to harm the accuracy of the evaporation process caused by the interruption by the physical presence of the thermometer. And this data is subsequently employed as the initial condition for the evaporation simulation.

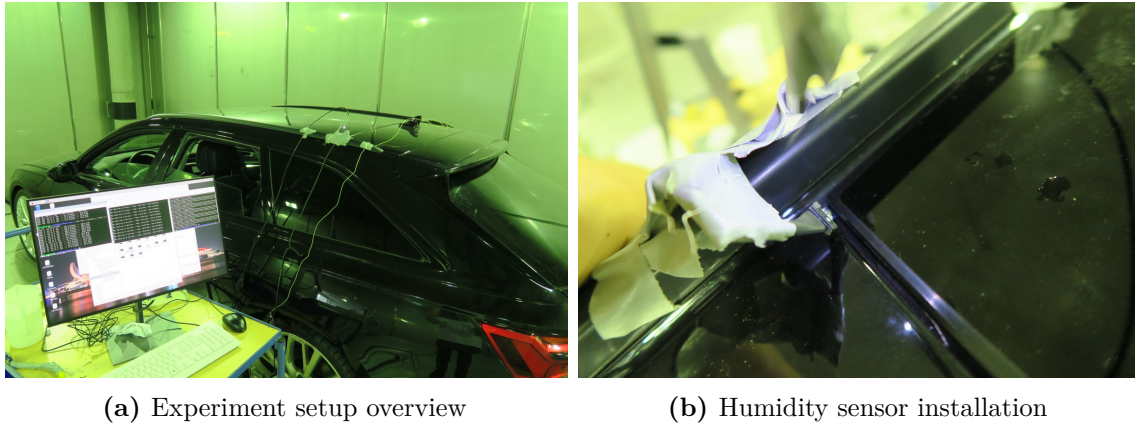


Figure 5.1: Experimental setup : An overview of the experimental setup inside of a climate chamber (left) and the installation of a humidity sensor (right) . Adopted from [LEE ET AL. 2024].

These sensors and endoscope are connected to a Raspberry Pi via either I2C or USB interface. The data values read into Raspberry Pi are then recorded in regular intervals, around 1 minute, so that they can be used for further analysis.

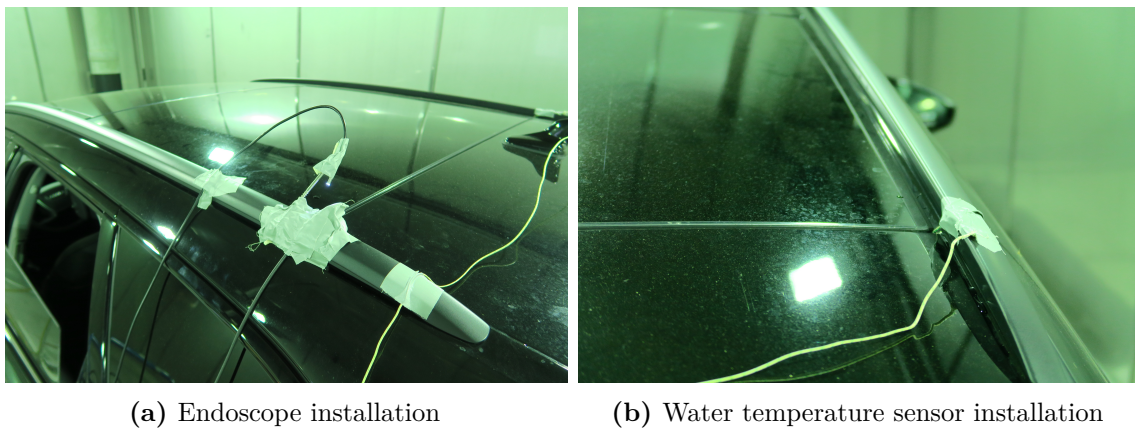


Figure 5.2: Experimental setup: Endoscope to capture the water source tracking over time (left) and the installation of a thermometer for water body temperature measurement (right).

The dry-out times are assessed under four distinct ambient conditions. As one example of the measurement cases, Figure 5.3 and Figure 5.4 illustrate the humidity sensor readings and water body temperature sensor readings over time, respectively. As indicated by the red line in the figure, the convergence of the sensor value to the ambient relative humidity signifies that the water accumulation is totally evaporated. It should be noted that the red lines in the figures mark the time point at which the deviation of the quantity stabilizes, with no further deviations exceeding 10%.

Additionally, the progression of the drying-out process is visually observable in the snapshot photos depicted in Figure 5.5, where the water is entirely evaporated in this specific area.

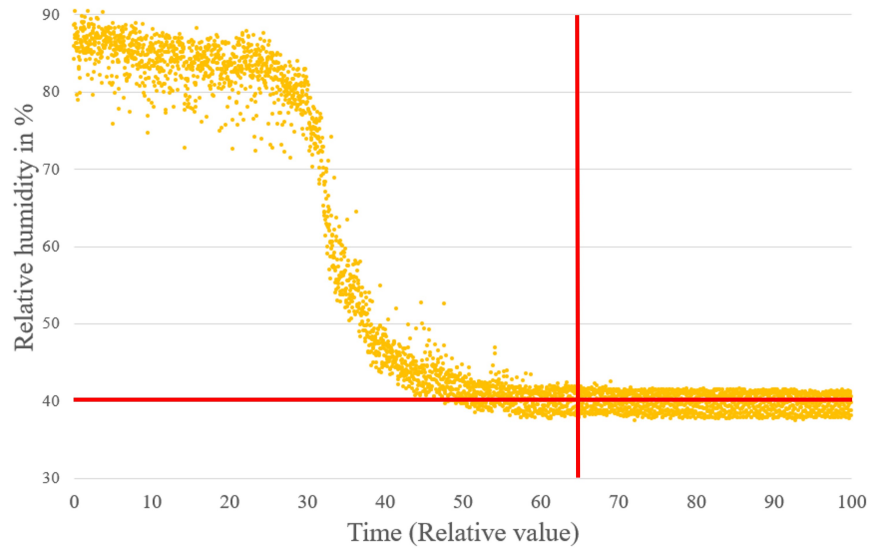


Figure 5.3: Experimental result example: Relative humidity sensor value readings over time. Adopted from [LEE ET AL. 2024].

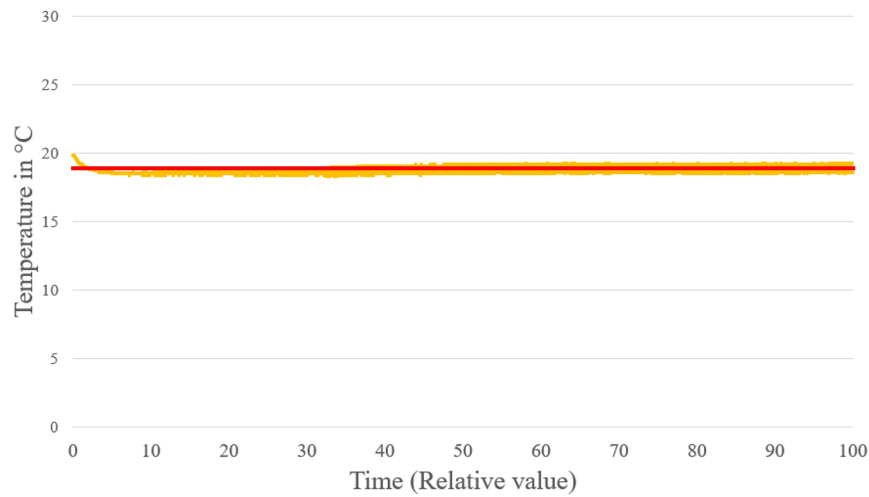


Figure 5.4: Experimental result example: Water body temperature sensor value readings over time.

By employing these inspection methods, the total dry-out times under varied ambient conditions are measured and subsequently used for validation of the simulation method.

5.1.2 Numerical simulation results

In order to first obtain the water accumulation, which would be the initial water source to be evaporated in the evaporation simulation, a preliminary raining simulation should be conducted as in Figure 5.6a, noting that the raining source is restricted so that it is sufficient to wet the components of interests for the sake of computational efficiency.



(a) Initial time



(b) Final time

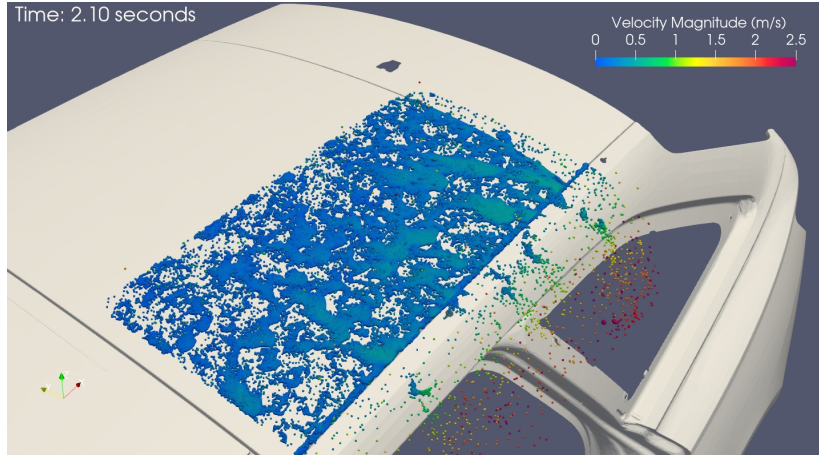
Figure 5.5: Snapshot examples of the leftover water at the corner of the sunroof channel: Initial state (top) and final state (bottom). Adopted from [LEE ET AL. 2024].

After the rain source is turned off, the simulation is left running as it is for a sufficient duration so that the water can be freely drained away from the body of the vehicle. Thus, only the water source at the corner of the sunroof channel is left based on the geometric formation of the region. This is subsequently used as the initial condition for the evaporation simulation as illustrated in Figure 5.6b.

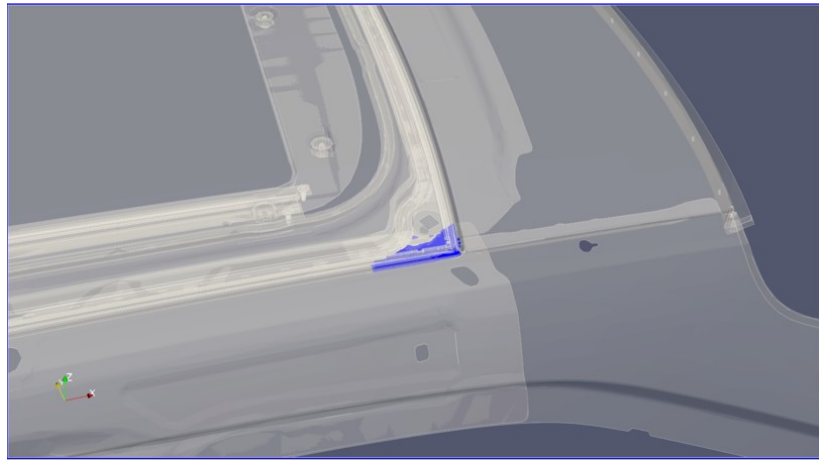
Evaporation rate acceleration

The resulting relative humidity profile, which is developed from the above-explained initial condition after some time, or also named as “startup time” (5s), is shown in Figure 5.7. Note that the ambient relative humidity is 60%.

Here, each phase is presented in separate pictures. The upper picture shows the relative humidity profiles, whereas the lower picture shows the extracted leftover water phase volume at 5s, noting that these profiles are from one monolithic multi-phase simulation. As depicted in the figure, the vapor propagates along the channel well from the water



(a) An example of raining simulation with GFDM



(b) Initial water source for the evaporation simulation

Figure 5.6: An example of raining simulation in order to obtain initial water source for the evaporation simulation (top) and initial water source after drainage for the evaporation simulation (bottom).

accumulation, and the vapor concentration profile stays fairly static, especially around the exposed free surface regions.

Furthermore, the simulated evaporation rate reaches a quasi-steady state with some tiny fluctuations after approximately 5s as depicted in Figure 5.8, which shows the integrated evaporation rate over time. Thus, under these observed circumstances, the calculated evaporation rate can be artificially accelerated with a time-lapse factor in order to extend the simulations time scale into real-world time scale and to effectively approximate the actual dry-out time [LEE ET AL. 2024].

The simulation outcomes over time are shown in Figure 5.9. It should be noted that the initial state refers to the time step right after the aforementioned quasi-steady state, and the elapsed times are presented as relative values from that time on, with 100 indicating complete dry-out from the simulation.

Besides, to circumvent the singularity issue, which can lead to instability in the entire simulation when there remains only a tiny amount of water source to be evaporated,

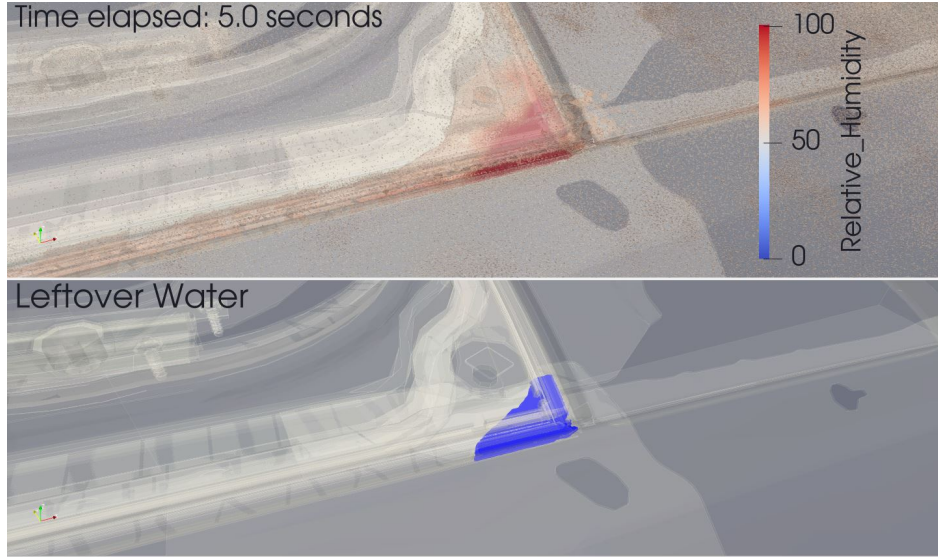


Figure 5.7: Vehicle A: Relative humidity profile (top) and the leftover water volume (bottom) of the evaporation simulation at 5s, shortly before to the acceleration.

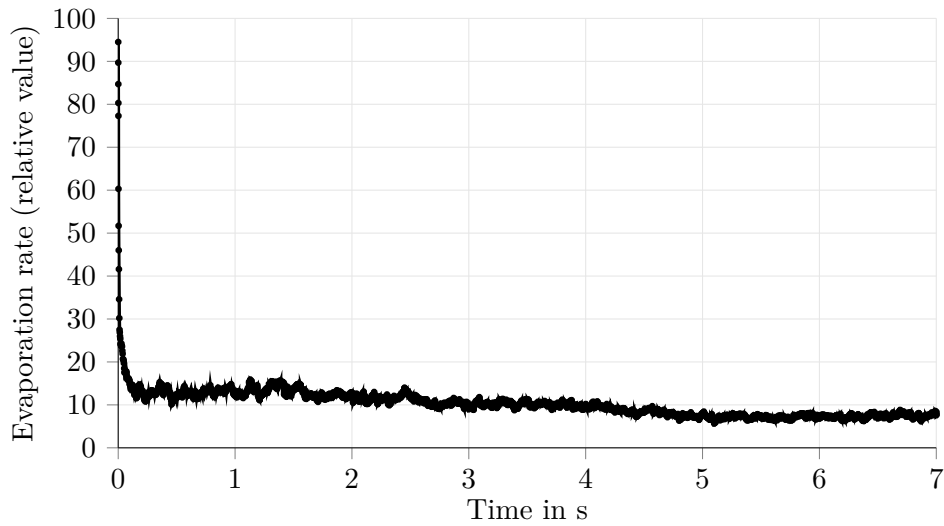
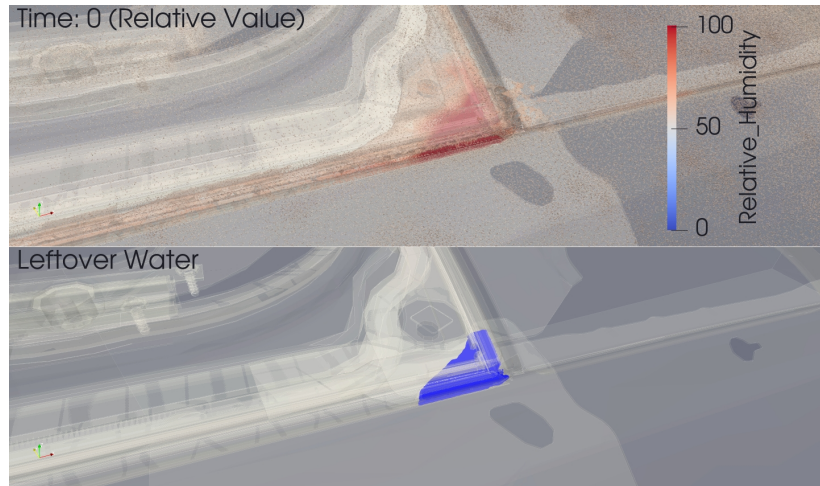


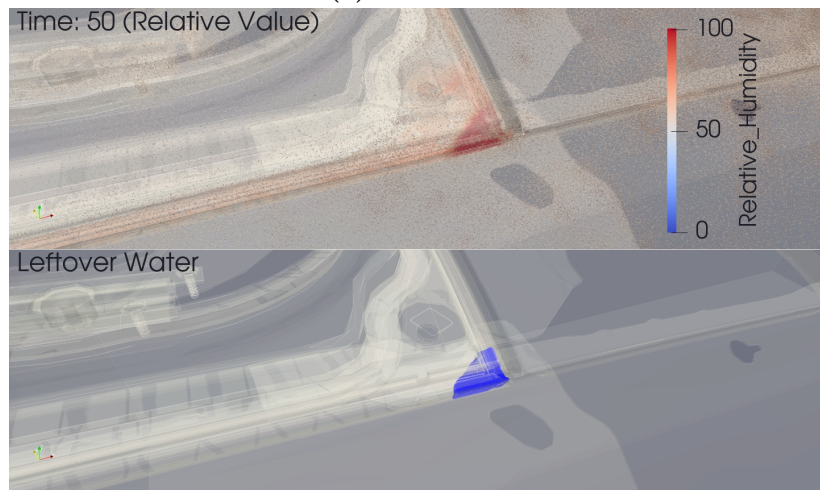
Figure 5.8: Simulation results: Evaporation rate over time the value reaches quasi-steady state after 5s of simulation time. Adopted from [LEE ET AL. 2024].

the simulation automatically terminates upon encountering extremely low water volume conditions or, more specifically 10^{-7} m^3 of water volume. The estimated dry-out time for this tiny amount of water, which is calculated from the evaporation rate and the leftover water amount at the last time steps, will then be added to the total dry-out time estimation [LEE ET AL. 2024].

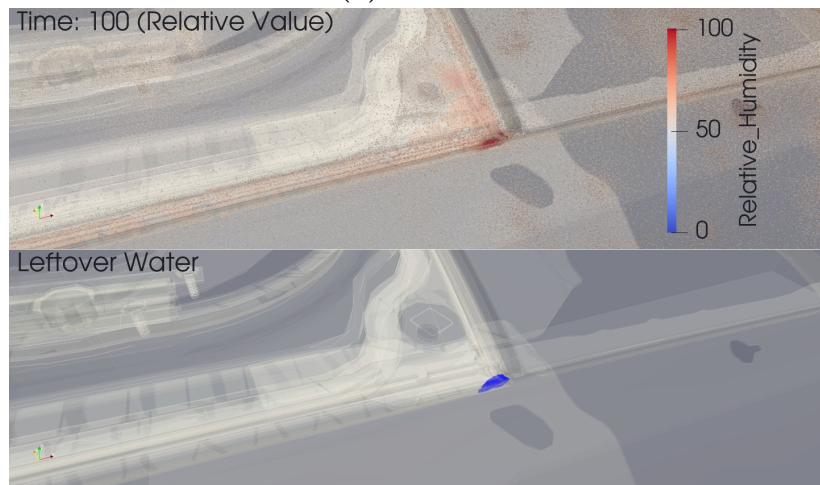
As illustrated in Figure 5.9, the gradual decrease in the remaining water quantity over time is observable in the simulation thanks to the introduced acceleration feature. Concurrently, the humidity profile in the region remains relatively constant, justifying the practical applicability of the acceleration approach.



(a) Initial time



(b) Mid time



(c) End time

Figure 5.9: Sunroof channel geometry (Vehicle A) simulation result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time). Adopted from [LEE ET AL. 2024].

Using the aforementioned methods, the simulation scenarios are executed under different ambient conditions as of the experiment. The comparisons of dry-out times are illustrated in Figure 5.10. In this context, the dry-out time is also presented in relative time values, where 100 denotes the total dry-out time from the simulation of the first case or the most extended evaporation duration case.

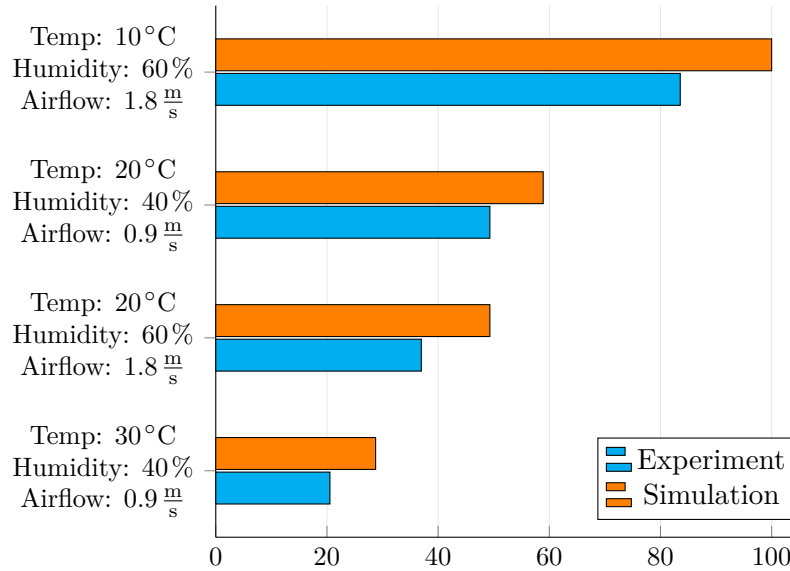


Figure 5.10: Validation result of vehicle A sunroof application the total dry-out time comparison (time in relative values). Adapted from [LEE ET AL. 2024].

Note that two cases (20°C with 40% and 30°C with 40%) were conducted in the first climate chamber, whose ventilation fan airflow rate is approximately 0.9 $\frac{m}{s}$. Whereas other two cases (10°C with 60% and 20°C with 60%) were performed in the second climate chamber with 1.8 $\frac{m}{s}$ airflow rate of ventilation facility.

Generally, the simulation results exhibit slightly longer dry-out times than the experimental results. This trend is to be expected as the estimated evaporation rates that are validated with a simple vessel in channel geometry cases (as in Section 4) yield lower evaporation rate values than the experimental results within the expected error.

In summary, the validation results demonstrate a satisfactory agreement with the experimental measurements, which is also acceptable from the corrosion protection measures point of view [LEE ET AL. 2024].

5.2 Sunroof channel geometry case for Vehicle B

(The majority of the contents in this section is already published in a conference [LEE ET AL. 2023b].)

In this section, a typical application of the developed method in the vehicle development process is introduced. Furthermore, like in the previous validation case, this new geometry in vehicle B is also validated under different ambient conditions.

5.2.1 Application for different component design variations in development process

During the vehicle development process, many different variations of design are introduced for one specific component, considering many mechanical aspects. In reality, it is not efficient at all or practically impossible to build all the candidate components for the desired tests, specifically dry-out time measurements in this current study. Thus, the developed method can be deployed in such scenarios.

As an example of such comparisons between the design variation situation, the corner of the sunroof channel of vehicle B, illustrated in Figure 5.11, is shown. Here, three distinct design variations of venting holes, as depicted in Figure 5.12, are introduced for this geometry.

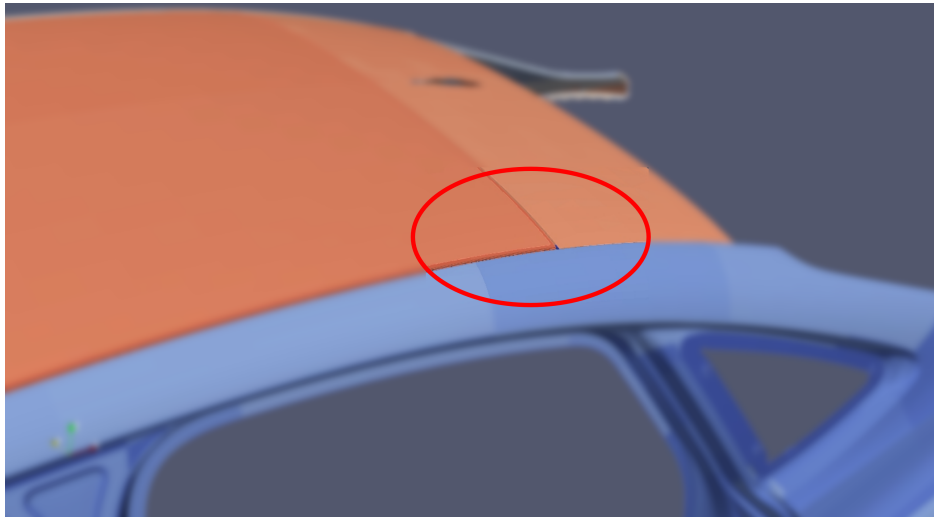


Figure 5.11: The sunroof channel region of Vehicle B. The rest are intentionally blurred.

Design variation 1 has a big venting hole, which is located slightly offset from the very corner. Variation 2 has a big venting hole at the exact corner of the sunroof channel geometry. Variation 3 has the smallest venting hole at the corner.

As previously explained in Section 5.1, the raining simulation is used in order to obtain a water source as the initial state for each design variation. The simulation is run for approximately 5s to achieve reasonable vapor propagation as well as a quasi-steady

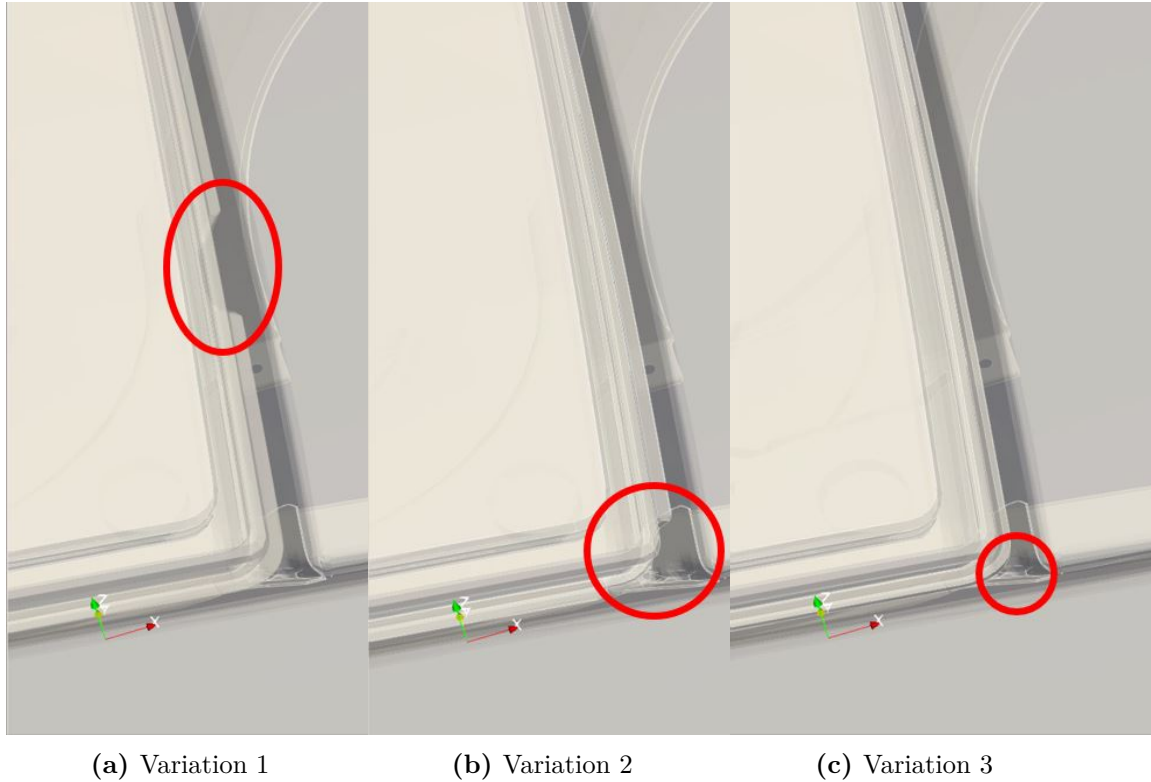


Figure 5.12: Three different component design variations for the corner of the sunroof channel. Adopted from [LEE ET AL. 2023b].

state evaporation rate over the exposed surface. Following that, the evaporation process is artificially accelerated to extend the simulation time scale.

The simulation results with each design variation are illustrated in Figure 5.13. Each pair of images displays the relative humidity profile (top) and the remaining water source (bottom). Each row corresponds to (a) the initial time, (b) Time = 50, (c) Time = 62, and (d) Time = 100. The simulated dry-out times are expressed in relative values, with 100 indicating the simulated total dry-out time with design Variation 3, which takes the longest time to dry.

Variation 1 experiences the shortest drying time (50% shorter time than the most extended variation) since it has the largest venting hole, which is not entirely blocked by the water accumulation, allowing air circulation inside the sunroof geometry. Variation 2, with a medium-sized venting hole, requires 62% of the total dry-out time of Variation 3. Variation 3 takes the longest time to dry out as it has the smallest venting hole, which makes physical sense.

From the simulation result, it is clearly demonstrated that the new method effectively captures the characteristics of various component design variations and accurately estimates the dry-out time. Consequently, these results can be applied to develop efficient corrosion protection schemes.

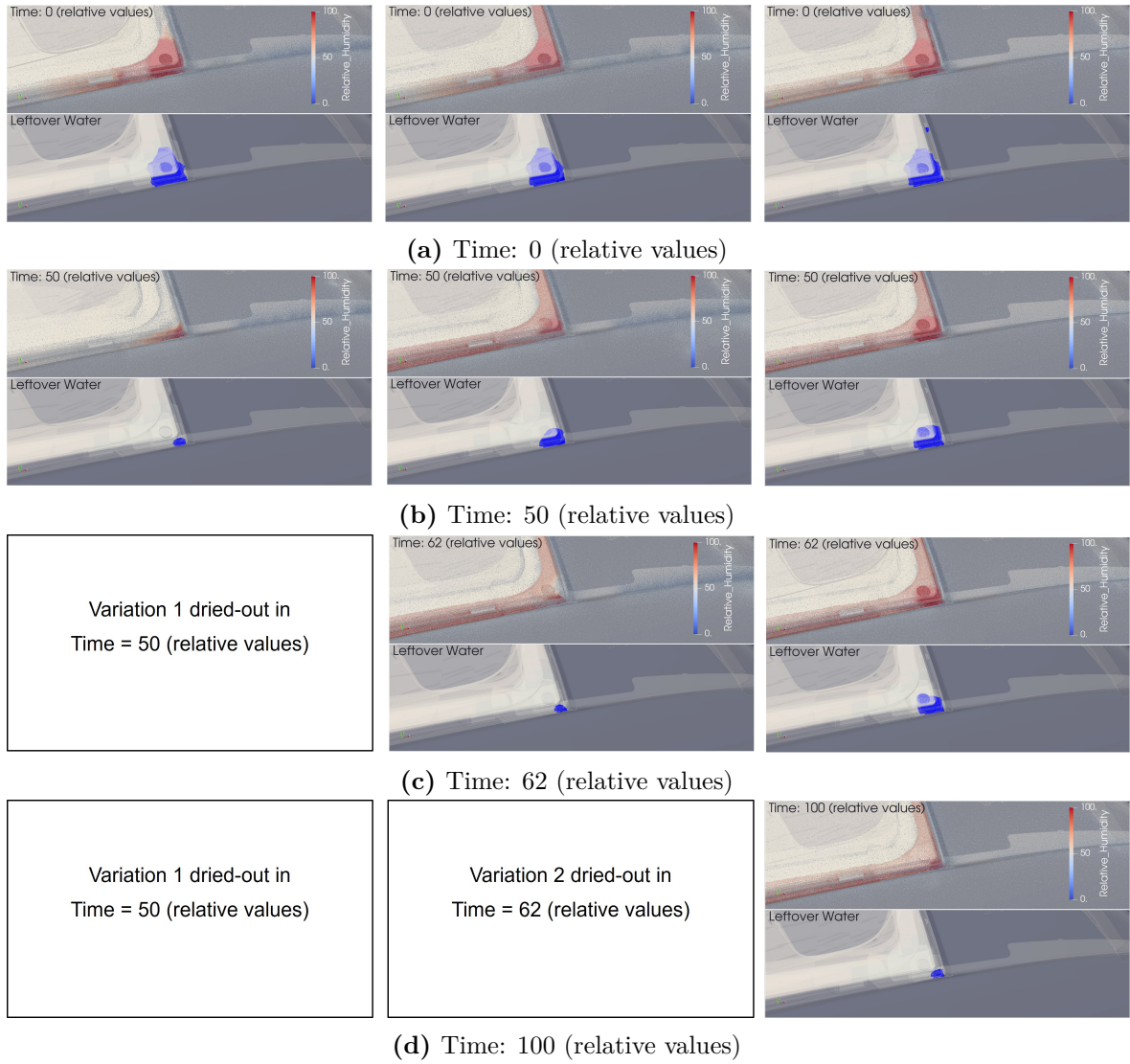


Figure 5.13: The simulated evaporation process over time with different design variations of the corner of the sunroof channel of vehicle B. In each time and variations, the relative humidity profile (upper) and the leftover water amount (bottom) are shown. The total dry-out time is 50 for Variation 1, 62 for Variation 2 and 100 for Variation 3, noting that time is in relative values . Adopted from [LEE ET AL. 2023b].

5.2.2 Experiment setup

Among the design variations in the previous application case, the actual geometry for the corresponding component deployed for the vehicle B is Variation 3. With this geometry, the dry-out time of the water accumulation at the corner of the sunroof channel is measured with a practically identical experiment setup as previously explained in Section 5.1.1.

The overview of the experimental setup and the installations of the humidity sensor and water body temperature sensor for the second vehicle are illustrated in Figure 5.14.



(a) Humidity sensor and endoscope installation



(b) Water temperature sensor installation

Figure 5.14: Experimental setup: The installation of a humidity sensor and a endoscope(top), and the water temperature sensor installations (bottom). Some parts of the photos are intentionally blurred.

The total dry-out times are measured under three different ambient conditions. Figure 5.15 demonstrates the humidity sensor values over time for the first measurement case. Similar to the results of the previous experiment (Section 5.1.1), the humidity sensor value converges to the ambient relative humidity value, which is indicated by the red line in the figure. This represents that the water accumulation in this region is totally evaporated.

Moreover, the dry-out progress over time is visually observable via endoscope snapshots as illustrated in Figure 5.16. Thus, the total dry-out time in this specific region can be approximated.

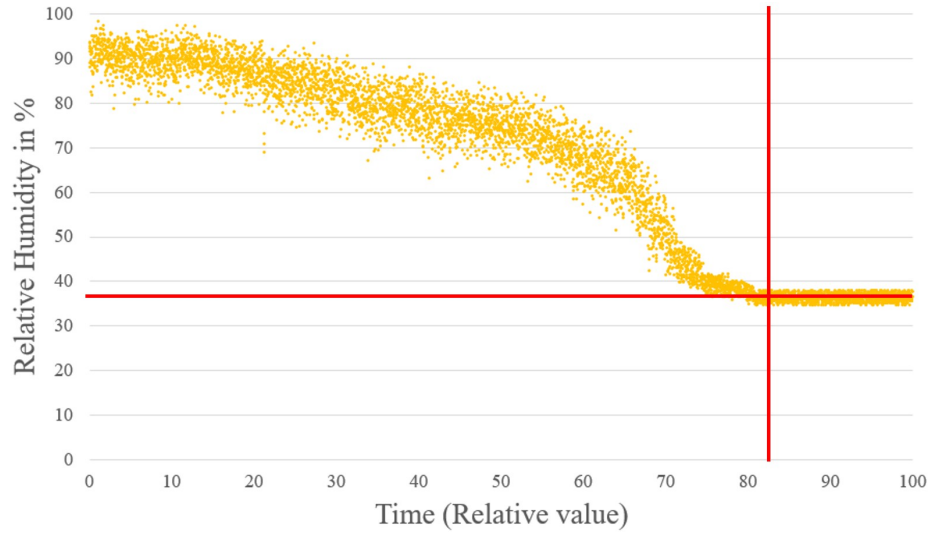
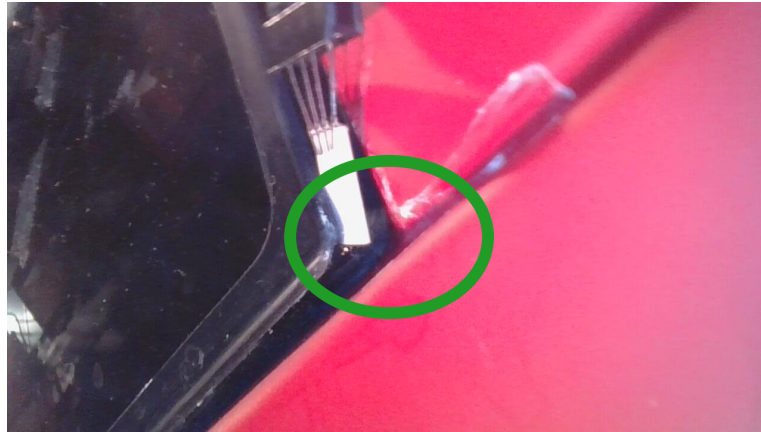
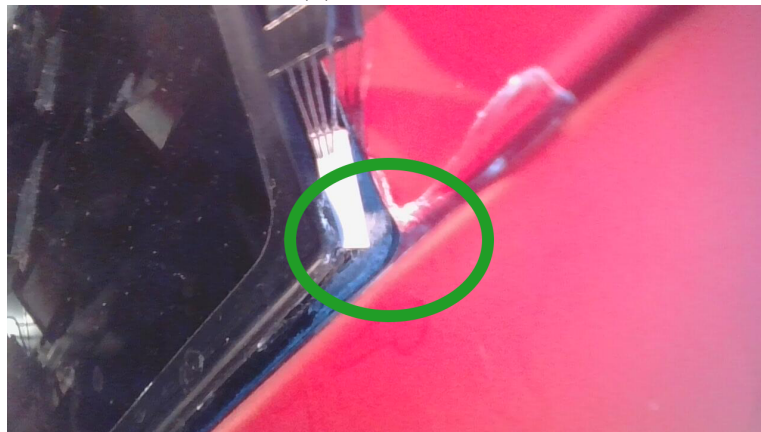


Figure 5.15: Experimental result example: Relative humidity sensor value readings over time.



(a) Initial time



(b) Final time

Figure 5.16: Snapshot examples of the leftover water at the corner of the sunroof channel: Initial state (top) and final state (bottom).

5.2.3 Numerical simulation results

Like in the vehicle A case (Section 5.1.2), a raining simulation was first deployed in order to obtain the initial water accumulation for the evaporation simulation. Following that, a quasi-steady state evaporation rate and humidity profile can be achieved after approximately 5s as depicted in Figure 5.17. Here, the upper picture describes the relative humidity profile, and the lower picture shows the leftover water volume.

Once this status is achieved, the evaporation phenomenon is then artificially accelerated with the scheme, which is thoroughly explained in Section 5.1.2.

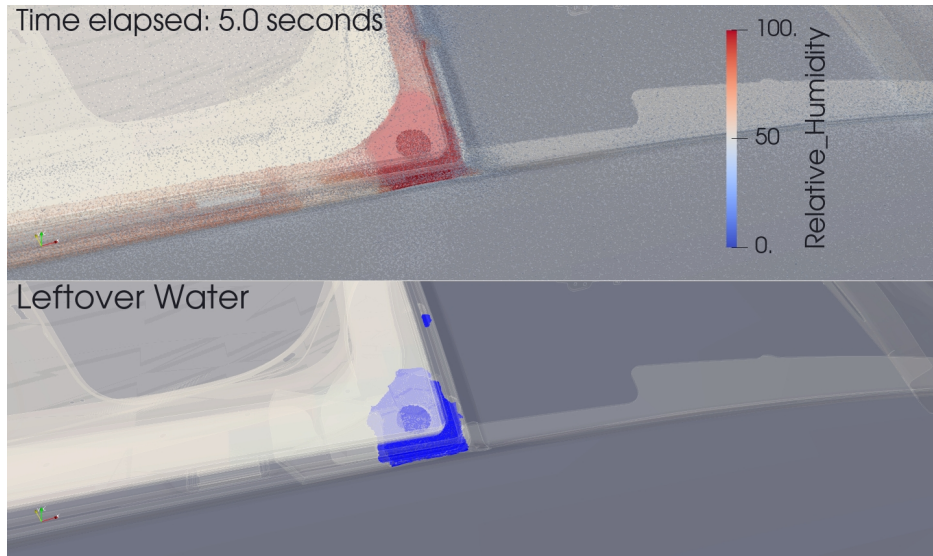
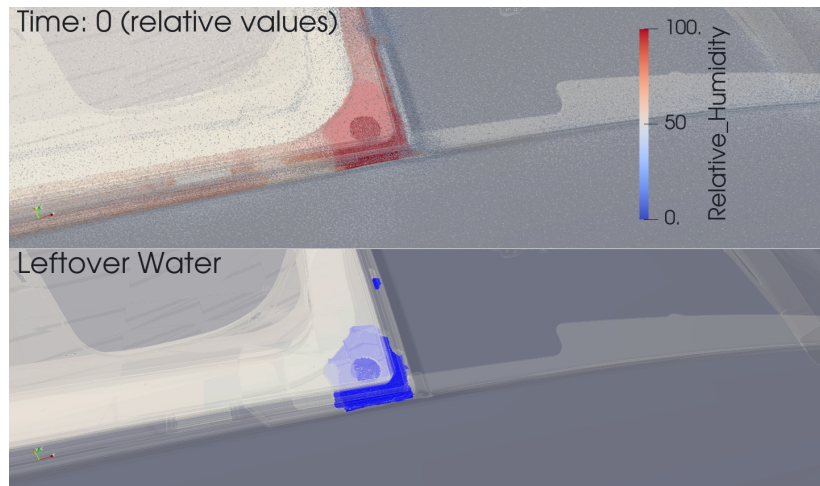


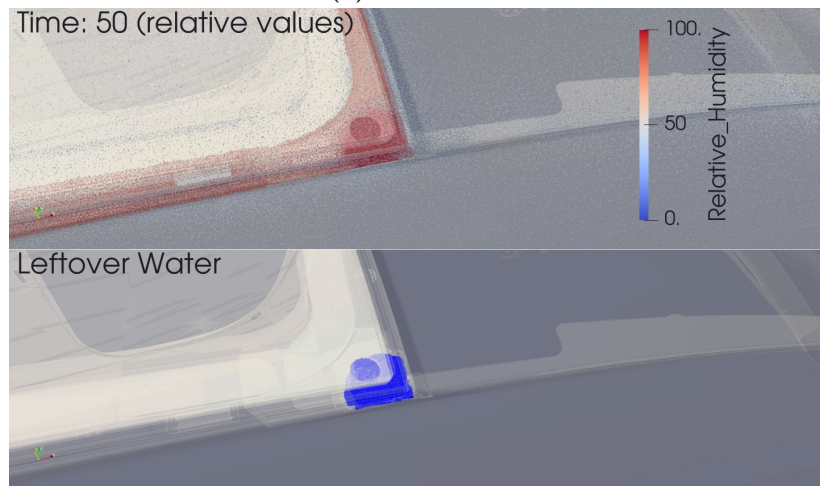
Figure 5.17: Vehicle B: Relative humidity profile (top) and the leftover water volume (bottom) of the simulation at 5s, shortly before to the acceleration.

The simulation outcomes with the acceleration are illustrated in Figure 5.18. It is clearly seen that the amount of water volume reduces gradually over time whereas the humidity profile around the water source is reasonably static. This, once again, makes sound reasoning for the application of the artificial acceleration scheme. In this context, the elapsed times are represented in relative value, where 100 indicates complete evaporation in this particular case. The simulation automatically halts upon encountering extremely low water volume conditions to avoid any instability in singularity situations.

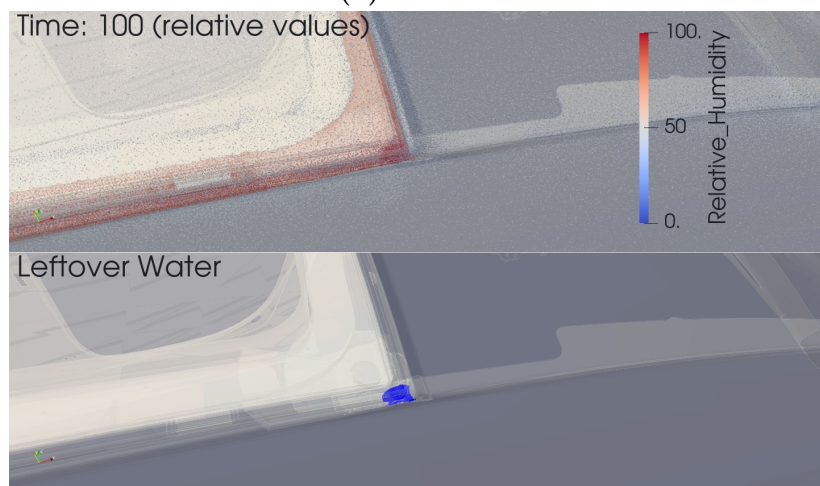
The validation results with the comparison of dry-out times under three distinct ambient conditions are demonstrated in Figure 5.19. Here, the dry-out times are represented in relative values, where 100 denotes the total dry-out time that is calculated from the simulation of the first case or the case that takes the maximum duration. The simulation outcomes show reasonably acceptable agreement with the experimental results and, especially, follow the trend excellently. In this validation case as well, the simulation results display slightly longer dry-out times than that of the experimental results in general, as expected from the previous validations (see Section 4).



(a) Initial time



(b) Mid time



(c) End time

Figure 5.18: Sunroof channel geometry (Vehicle B) simulation result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time).

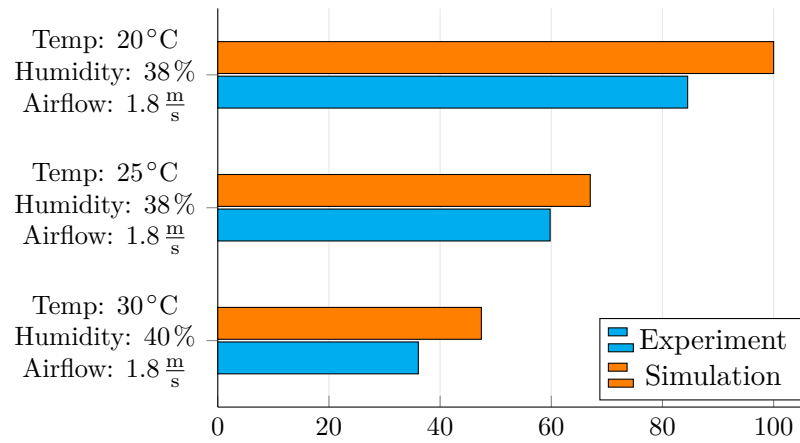


Figure 5.19: Validation result of vehicle B sunroof application the total dry-out time comparison (time in relative values).

In conclusion, the application and validation of the developed method in the case of vehicle B were also successfully performed.

6 Further applications

The newly developed method is successfully applied to vehicle sunroof channel geometries and validated in this thesis. In this chapter, further potential improvement points with application examples are introduced in order to enhance the method as an example of further applications.

6.1 Application to more sophisticated vehicle geometries

First of all, investigation and validation of the method for more sophisticated and comprehensive vehicle geometries should be performed. One example of such applications is the high-voltage battery housing geometry in electric vehicles, as illustrated in Figure 6.1.

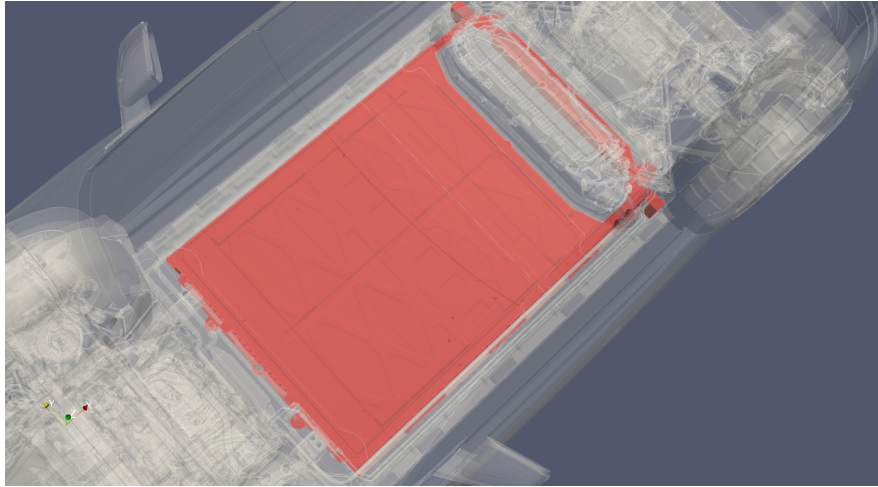


Figure 6.1: Battery housing region (denoted as red) of a electric vehicle. The rest parts are intentionally blurred.

When the vehicle traverses a water reservoir or encounters water-wading scenarios, water may penetrate the flat battery gap region, as shown in the water-wading simulation results illustrated in Figure 6.2. Here, the upper picture shows the entire water volume simulated, and the bottom picture shows only the clipped region of interest.

Assuming that the rest of the water around this battery housing gap region drains away shortly after the wading, the developed dry-out simulation can be deployed with the initial water accumulation status obtained from the previous wading simulation. Similar to the previous sunroof channel cases, the dry-out simulation is run initially for

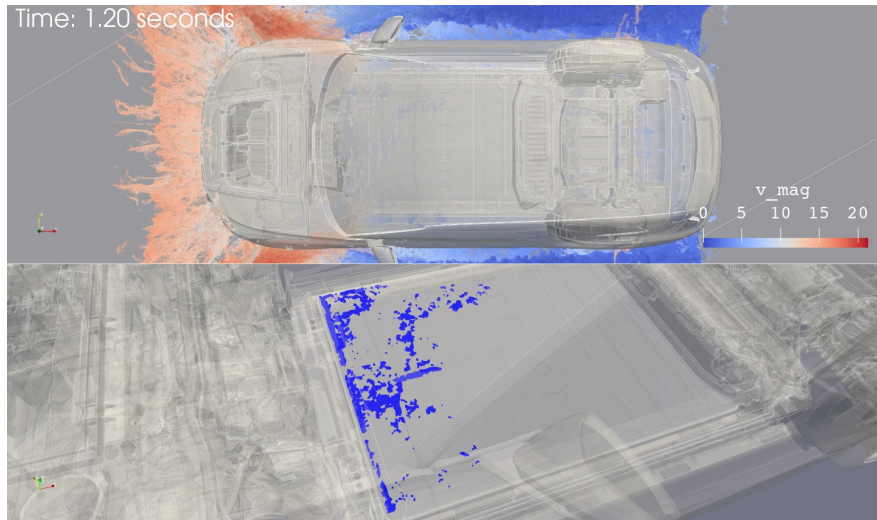


Figure 6.2: Water wading simulation results. An overview showing entire water volume in the simulation domain (top), and clipped view of the water volume intrude into the battery housing region (bottom). Some parts of the pictures are intentionally blurred.

some time (or “startup time”) without evaporation rate acceleration as presented in Figure 6.3.

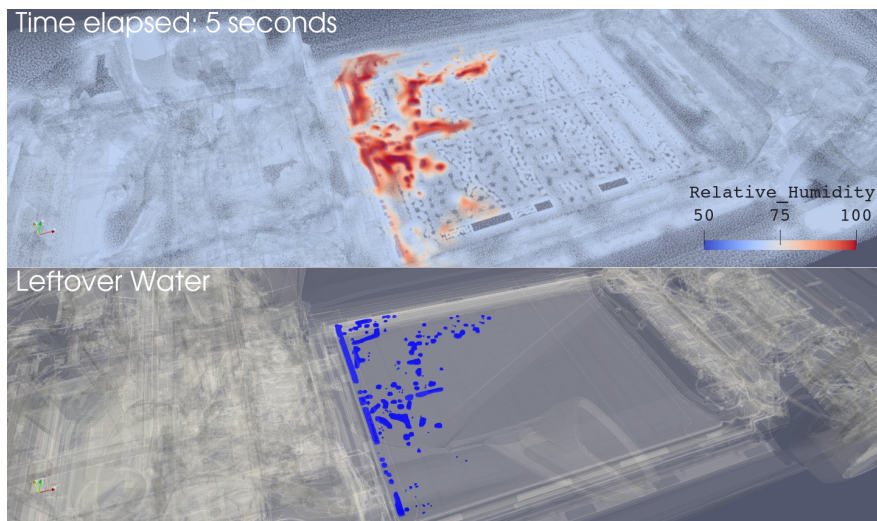
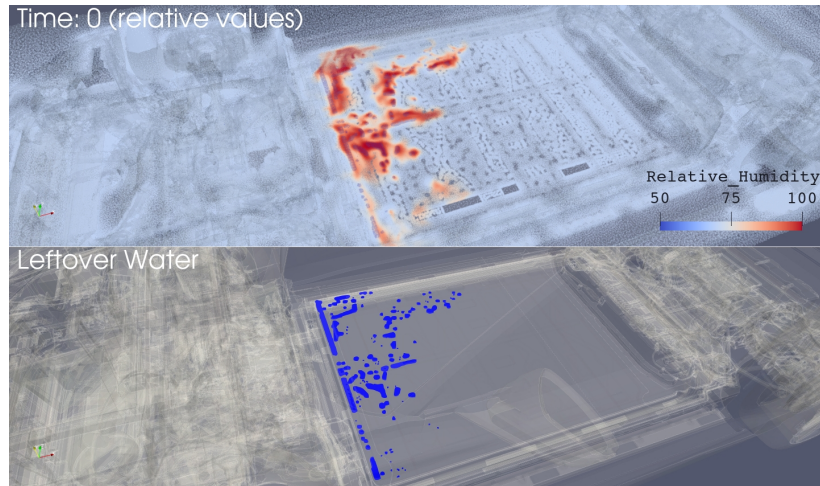
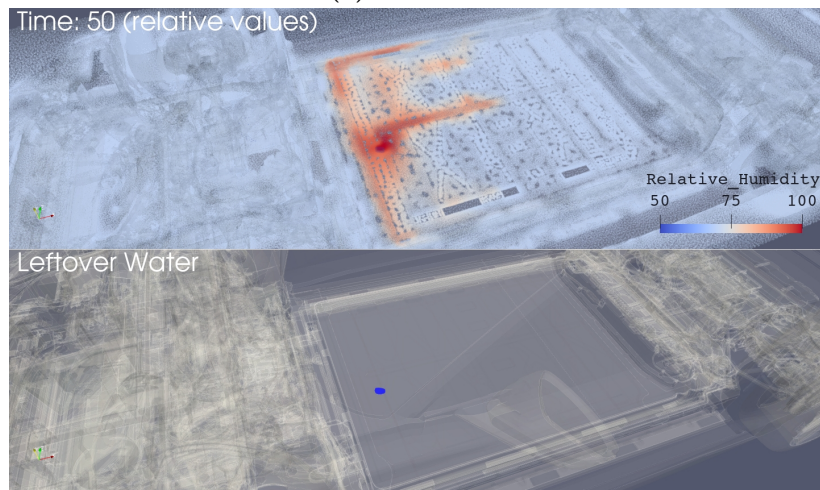


Figure 6.3: Battery housing region: Relative humidity profile (top) and the leftover water volume (bottom) of the evaporation simulation at 5s, shortly before to the acceleration applied.

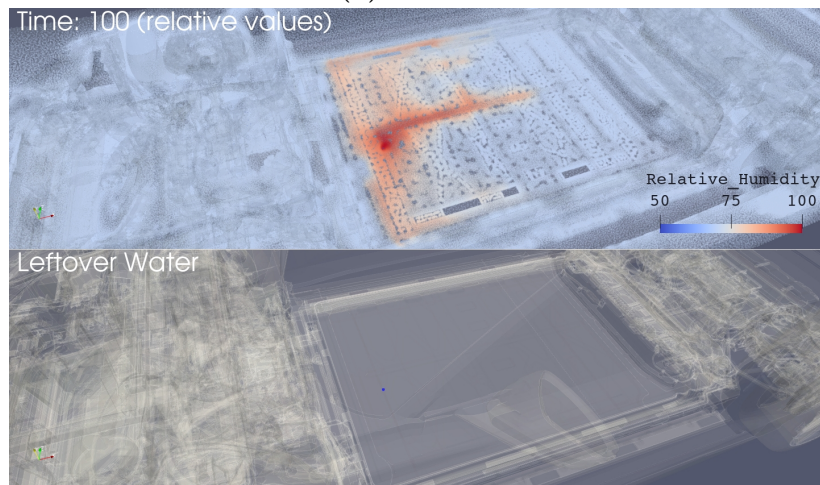
The dry-out process is accelerated from this startup time on with the given time-laps factor. The results of the dry-out simulation are depicted in Figure 6.4, where the time elapsed is shown in relative value. The water source in the middle of the gap takes the longest time to evaporate since the vapor generated from the droplets accumulates around this region without proper ventilation. However, most of the wet parts of the gap dried out relatively fast, even before half of the total dry-out time from the simulation outcomes.



(a) Initial time



(b) Mid time



(c) End time

Figure 6.4: Battery region simulation result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time).

This further application example shows that the method could be applied to more sophisticated and larger vehicle components. Nevertheless, further investigations are required in order to efficiently deploy these applications. First, when the computation domain becomes on a much larger scale, strategies to find an optimal minimum smoothing length criteria (or finest refinement) are essential.

Even if the automatic adaptive refinement works well in such cases as well, it sometimes extensively refines to capture every detail of surrounding parts or edges, which would generate an enormous number of points. Thus, the simulation runtime and required number of computing nodes would explode in such cases. Furthermore, more validation should be performed for such larger and more complex geometric formations.

6.2 Application of the thermal effects of vehicle components

Another potential improvement point would be adapting and validating the thermal effects of the vehicle components. For the mechanical and electrical components of the vehicle, it is common for the parts to be heated up and become warm during the operation. Furthermore, when an EV is in charge, the battery also warms up.

In order to take into account such thermal effects on the dry-out process, a stable simulation solution is required even with various temperature boundary conditions. As an example of such cases, a warmed-up battery scenario is tested with fixed-value Dirichlet BC on the battery component, assuming that the battery is heated up during charging as illustrated in Figure 6.5.

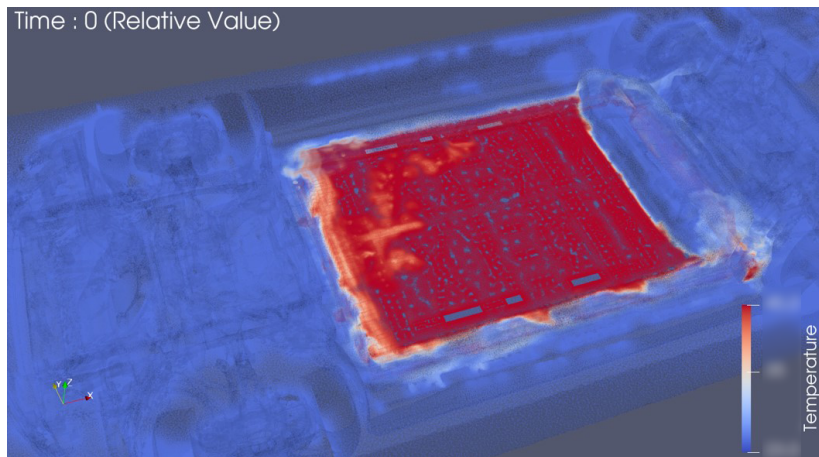
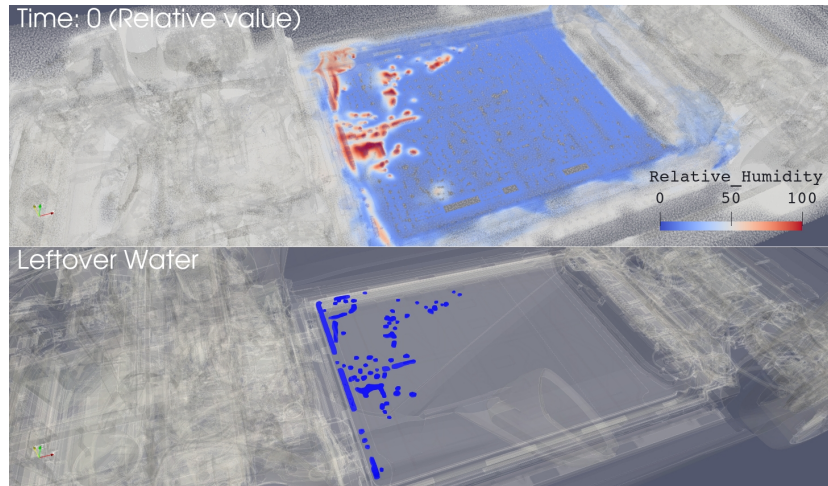
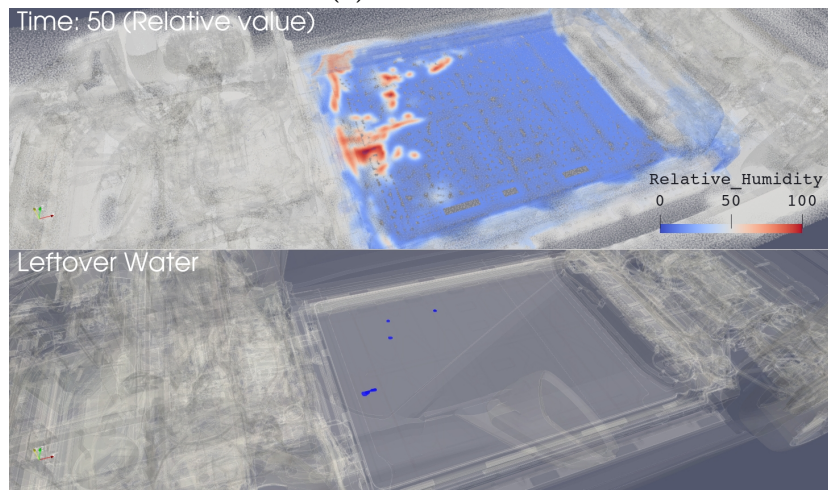


Figure 6.5: Temperature profile of the simulation at 5s, shortly before to the acceleration. The values are blurred intentionally.

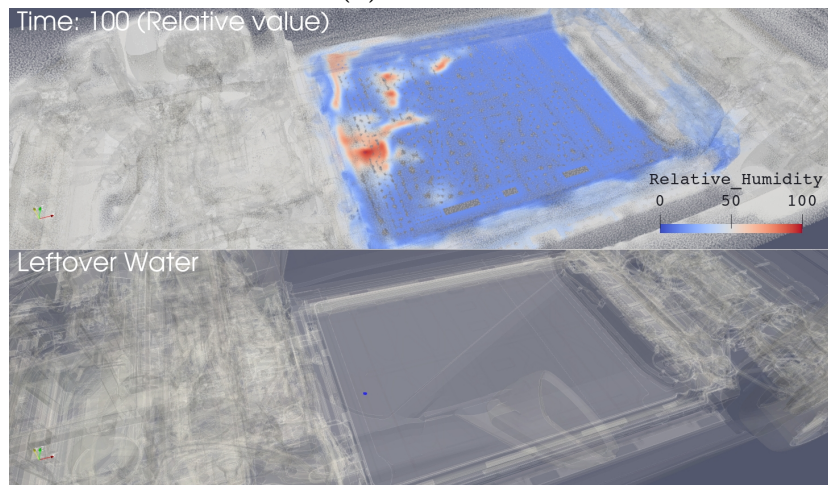
The simulation runs stably with the identical Dirichlet temperature BC for both phases, as shown in Figure 6.6. It should be noted that the relative humidity values are lower than the ambient around the battery housing gap due to higher temperatures in this region.



(a) Initial time



(b) Mid time



(c) End time

Figure 6.6: Battery region simulation with Dirichlet thermal boundary condition result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time).

This test example presents that the method is applicable and runs stably with Dirichlet thermal BCs with a relatively small temperature difference, approximately 20°C . In order to simulate further scenarios accurately, more investigations, including the application of heat flux BCs (Neumann thermal BCs) and larger temperature difference cases, are required. Moreover, the validation procedure with thermal effects should also be performed.

7 Conclusion

This research aimed to construct a robust numerical method to resolve below-boiling point evaporation physics and consequent dry-out time of wet vehicle components. New models to deal with the evaporation phenomena are implemented in the traditional FVM with VoF model (OpenFOAM) and in a GFDM meshfree collocation approach (MESHFREE). Within the GFDM, three different versions are introduced: a simplified single-phase, multi-phase with the surface-surface-coupling, and multi-phase with the volume-volume-coupling.

In order to validate all the implemented models, an experiment with a relatively simple geometry to measure the evaporation rate for different airflow rates, ambient temperatures, and ambient relative humidities is designed and built. A thorough validation is performed by comparing all the measurement points with the numerical simulation outcomes. The multi-phase approaches presented good correlations to the experiment, whereas the single-phase results showed more significant but acceptable deviations.

In the GFDM approaches, along with the new model, an automatized adaptive refinement feature based on the humidity- and velocity-gradients is developed by adapting one of the most significant advantages of the meshfree method over traditional FVM. The computation time could be optimized through this new feature, giving more flexibility to the solver so that it can be easily applied to arbitrary geometries.

Among the investigated approaches, GFDM volume-volume-coupling is proven to be the best approach for the purpose of this study based on criteria such as accuracy, flexibility, and stability. Thus, this approach is deployed for further application to actual vehicle geometries and validations.

For further investigation, the total dry-out times of an accumulated water source at the corner of the sunroof channel of two different vehicles are measured under different ambient conditions. In order to extend the simulation time scale to a real-world time scale, the evaporation rate or the water amount reduction rate is artificially accelerated once it reaches a quasi-steady state. With this technique, the total dry-out time could be practically approximated. The validation outcomes with actual vehicle applications presented acceptable total dry-out time approximations. The simulation results closely followed the experimental trends, indicating a strong agreement. This consistency underscores the reliability of the simulation method in predicting real-world performance.

In addition, a typical applicational case of the method for vehicle component design variations is demonstrated as a showcase of its deployment during the vehicle development phase. The simulation outcomes are promising, as the method effectively captures

the attributes of different component designs and predicts the associated dry-out time. The simulation outcomes are promising as the method effectively captures the attributes of different component design variations and predicts the associated dry-out time. Ultimately, these findings can guide effective component designs for better corrosion protection schemes.

Then, two potential improvements to the method are presented as examples of further applications, supported by example simulations to illustrate their impact. First, a deeper investigation of the effective deployment of the method to more sophisticated and comprehensive vehicle geometries is required in order to find optimal refinement criteria. Second, as temperature is one of the major conditions that highly affects the dry-out time result, advanced studies to run the simulation stably, even with various thermal effects such as different thermal boundary conditions and large temperature differences, should also be conducted.

In conclusion, the research introduced in this study presented a robust and comprehensive solution to predict the total dry-out time of wet vehicle components and gave more possibilities to extend the CFD technique in the automotive sector's water management applications.

List of Tables

4.1	Runtime comparison for 5s of simulation time for different airflow rates, 20.5°C air temperature, and approximately 60% relative humidity. Partly adapted from [LEE ET AL. 2023a].	80
4.2	Comparison of simulations and experiments: Relative error of the numerical evaporation rates with respect to the experimental data for the 1.0 $\frac{m}{s}$ airflow rate. The highlighted values indicate that the simulation error is larger than the measurement uncertainty. Partly adapted from [LEE ET AL. 2023a].	82
4.3	Comparison of simulations and experiments: Relative error of the numerical evaporation rates with respect to the experimental data for the 1.8 $\frac{m}{s}$ airflow rate. The highlighted values indicate that the simulation error is larger than the measurement uncertainty. Partly adapted from [LEE ET AL. 2023a].	83
4.4	Comparison of simulations and experiments: Relative error of the numerical evaporation rates with respect to the experimental data for the 2.7 $\frac{m}{s}$ airflow rate. The highlighted values indicate that the simulation error is larger than the measurement uncertainty. Partly adapted from [LEE ET AL. 2023a].	84

List of Figures

1.1	Wet surfaces of vehicle example	1
3.1	Temperature vs. specific volume diagram at 1atm. Adapted from [ÇENGEL ET AL. 2016].	14
3.2	Localized corrosion illustrations. Adapted from [ROBERGE 2008].	16
3.3	Domain discretization with two point clouds for the single-phase simulations. The color indicates different types of points: interior points (blue), free surface points (red), and wall boundary points (white). Only a clip of the full point cloud is shown. Adopted from [LEE ET AL. 2023a].	22
3.4	Domain discretization with a point cloud for the multi-phase simulations. The color indicates the different phases: air phase (blue) and water phase (red). Points of both phases are present at the interface, marked with lighter shades of blue and red, respectively. This figure shows the surface-surface-coupling case as an example. Adopted from [LEE ET AL. 2023a].	22
3.5	Different volume definition of point cloud. Adapted from [SUCHDE ET AL. 2023].	34
3.6	Point cloud organization examples of the non-overlapping surface-surface-coupling (left) and the overlapping volume-volume-coupling (right). Adopted from [LEE ET AL. 2024].	40
3.7	Singularity issue with GFDM approach when extremely small water volume is left. Water free surface is shown in 3D and air phase shows clipped image perpendicular to the water droplet.	43
3.8	Domain discretization with non-overlapping finite volume elements example in 2D cross-section view with meshing around a vessel element. Upper figure includes the vessel geometry and the lower figure only shows generated mesh.	45
3.9	PIMPLE algorithm flow chart.	52
3.10	Example of the α field representation of each cell in two-phase flow.	53
3.11	PIMPLE algorithm flow chart with comprehensive equation set.	56
4.1	Schematic view of the evaporation rate measurement experiment. Detailed dimensions of the actual experiment geometry are demonstrated in Section 4.1 as well as in Figure 4.6. Adopted from [LEE ET AL. 2023a].	60
4.2	Experimental setup: Four EBM Papst 8212 JN axial fans at the channel outlet to generate constant airflow. Adopted from [LEE ET AL. 2023a].	61
4.3	Experimental setup: Mesh structures at the channel inlet to reduce turbulence. Adopted from [LEE ET AL. 2023a].	61

4.4	Experimental setup: Structure inside the channel. Adopted from [LEE ET AL. 2023a].	62
4.5	Experimental setup: Channel and climate chamber. Adopted from [LEE ET AL. 2023a].	62
4.6	Bounding geometry matching the experimental setup (channel, sensors, and vessel). The red-colored region indicates the initial water mass in the vessel. Adopted from [LEE ET AL. 2023a].	63
4.7	Mesh pre-processing overview for FVM simulation for the validation.	64
4.8	FVM simulation result: The initial state of VoF alpha field profile. The color indicates different types of phase: air phase(blue), and water phase (red). Only the cross section of the 3D domain is shown. Adopted from [LEE ET AL. 2022c].	64
4.9	FVM simulation result: Virtually constant vapor distribution within the domain over time – resulting in constant evaporation rate. Only the cross section of the 3D domain is shown. Adopted from [LEE ET AL. 2022c].	65
4.10	FVM multi-phase simulation result: Leftover water mass over time for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 40.6% relative humidity. Adapted from [LEE ET AL. 2022c].	65
4.11	Convergence study with respect to the number of cells for the $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 40.6% relative humidity.	66
4.12	FVM multi-phase simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2022c].	67
4.13	Water-only single-phase simulation result: Constant evaporation rate at the free surface points over time indicated by the color scale – identical evaporation rate profile for both 1s and 5s. Adopted from [LEE ET AL. 2023a].	69
4.14	Single-phase simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2023a].	71
4.15	Multi-phase simulation result with pre-defined regional refinement: Relative humidity profile from 0s to 5s in the cross section of the domain for $1.0 \frac{\text{m}}{\text{s}}$ airflow rate, 32.2°C air temperature, and 78% relative humidity. Adopted from [LEE ET AL. 2023a].	72
4.16	Multi-phase simulation result with pre-defined regional refinement: Evaporation rate over time for $1.0 \frac{\text{m}}{\text{s}}$ airflow rate, 32.2°C air temperature, and 78% relative humidity. Adopted from [LEE ET AL. 2023a].	73
4.17	Multi-phase simulation result with adaptive refinement refinement: Relative humidity profile from 0s to 5s in the cross section of the domain for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 57.3% relative humidity. Adapted from [LEE ET AL. 2022b].	74

4.18	Multi-phase simulation result with adaptive refinement with (black) and without (blue) startup time: Evaporation rate over time for $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.2°C air temperature, and 57.3% relative humidity. Adopted from [LEE ET AL. 2022b].	75
4.19	Convergence study with respect to the point cloud resolution for the $1.8 \frac{\text{m}}{\text{s}}$ airflow rate, 20.5°C air temperature, and 57.3% relative humidity. The bracketed values next to the marker points indicate the minimum point cloud resolution around the water-air interface. Adopted from [LEE ET AL. 2023a].	76
4.20	Surface-surface-coupling simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2023a].	77
4.21	Volume-volume-coupling simulation validation: Numerical vs. experimental evaporation rate for each airflow rate cases. The bracketed values next to the marker points indicate the equilibrium water body temperature. Adopted from [LEE ET AL. 2024].	78
5.1	Experimental setup : An overview of the experimental setup inside of a climate chamber (left) and the installation of a humidity sensor (right) . Adopted from [LEE ET AL. 2024].	88
5.2	Experimental setup: Endoscope to capture the water source tracking over time (left) and the installation of a thermometer for water body temperature measurement (right).	88
5.3	Experimental result example: Relative humidity sensor value readings over time. Adopted from [LEE ET AL. 2024].	89
5.4	Experimental result example: Water body temperature sensor value readings over time.	89
5.5	Snapshot examples of the leftover water at the corner of the sunroof channel: Initial state (top) and final state (bottom). Adopted from [LEE ET AL. 2024].	90
5.6	An example of raining simulation in order to obtain initial water source for the evaporation simulation (top) and initial water source after drainage for the evaporation simulation (bottom).	91
5.7	Vehicle A: Relative humidity profile (top) and the leftover water volume (bottom) of the evaporation simulation at 5s, shortly before to the acceleration.	92
5.8	Simulation results: Evaporation rate over time the value reaches quasi-steady state after 5s of simulation time. Adopted from [LEE ET AL. 2024].	92
5.9	Sunroof channel geometry (Vehicle A) simulation result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time). Adopted from [LEE ET AL. 2024].	93

5.10	Validation result of vehicle A sunroof application the total dry-out time comparison (time in relative values). Adapted from [LEE ET AL. 2024].	94
5.11	The sunroof channel region of Vehicle B. The rest are intentionally blurred.	95
5.12	Three different component design variations for the corner of the sunroof channel. Adopted from [LEE ET AL. 2023b].	96
5.13	The simulated evaporation process over time with different design variations of the corner of the sunroof channel of vehicle B. In each time and variations, the relative humidity profile (upper) and the leftover water amount (bottom) are shown. The total dry-out time is 50 for Variation 1, 62 for Variation 2 and 100 for Variation 3, noting that time is in relative values . Adopted from [LEE ET AL. 2023b].	97
5.14	Experimental setup: The installation of a humidity sensor and a endoscope(top), and the water temperature sensor installations (bottom). Some parts of the photos are intentionally blurred.	98
5.15	Experimental result example: Relative humidity sensor value readings over time.	99
5.16	Snapshot examples of the leftover water at the corner of the sunroof channel: Initial state (top) and final state (bottom).	99
5.17	Vehicle B: Relative humidity profile (top) and the leftover water volume (bottom) of the simulation at 5s, shortly before to the acceleration. . .	100
5.18	Sunroof channel geometry (Vehicle B) simulation result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time).	101
5.19	Validation result of vehicle B sunroof application the total dry-out time comparison (time in relative values).	102
6.1	Battery housing region (denoted as red) of a electric vehicle. The rest parts are intentionally blurred.	103
6.2	Water wading simulation results. An overview showing entire water volume in the simulation domain (top), and clipped view of the water volume intrude into the battery housing region (bottom). Some parts of the pictures are intentionally blurred.	104
6.3	Battery housing region: Relative humidity profile (top) and the leftover water volume (bottom) of the evaporation simulation at 5s, shortly before to the acceleration applied.	104
6.4	Battery region simulation result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time).	105
6.5	Temperature profile of the simulation at 5s, shortly before to the acceleration. The values are blurred intentionally.	106

6.6	Battery region simulation with Dirichlet thermal boundary condition result example: The relative humidity profile (top) and the leftover water (bottom) at each chosen time steps – Initial, mid, and the end time steps (relative time).	107
-----	--	-----

Bibliography

ANDERSON 1995

ANDERSON, J. D.: *Computational Fluid Dynamics*. 1st. New York: McGraw-Hill Education, 1995.

ANDERSON 2010

ANDERSON, J. D.: *Fundamentals of Aerodynamics*. 5th. New York: McGraw-Hill Education, 2010.

BAGHERI 2019

BAGHERI, M.: *Numerical Simulation of Evaporation to Assess Water Management Performance of Vehicles*. MA thesis. University of Rostock, 2019.

BLÁZQUEZ ET AL. 2017

BLÁZQUEZ, J. F.; MAESTRE, I.; GALLERO, F. G.; GÓMEZ, P. Á.: *A new practical CFD-based methodology to calculate the evaporation rate in indoor swimming pools*. *Energy and Buildings* 149 (2017), pp. 133–141. DOI: 10.1016/j.enbuild.2017.05.023.

BRENNEN 2005

BRENNEN, C. E.: *Fundamentals Of Multiphase Flow*. Cambridge University Press, 2005.

BROWN ET AL. 2001

BROWN, D. L.; CORTEZ, R.; MINION, M. L.: *Accurate Projection Methods for the Incompressible Navier–Stokes Equations*. *Journal of Computational Physics* 168.2 (2001), pp. 464–499. ISSN: 0021-9991. DOI: <http://dx.doi.org/10.1006/jcph.2001.6715>.

BUCK 1981

BUCK, A. L.: *New Equations for Computing Vapor Pressure and Enhancement Factor*. *Journal of Applied Meteorology and Climatology* 20 (1981), pp. 1527–1532. DOI: 10.1175/1520-0450(1981)020<1527:NEFCVP>2.0.CO;2.

ÇENGEL 2002

ÇENGEL, Y. A.: *Heat Transfer: A Practical Approach*. 2nd. New York: McGraw-Hill Education, 2002.

ÇENGEL & GHAJAR 2014

ÇENGEL, Y. A.; GHAJAR, A. J.: *Heat and Mass Transfer: Fundamental and application*. 5th. New York: McGraw-Hill Education, 2014.

ÇENGEL ET AL. 2016

ÇENGEL, Y. A.; TURNER, R. H.; CIMBALA, J. M.: *Fundamentals of thermal-fluid sciences*. 5th. McGraw-Hill Education, 2016.

ÇENGEL & CIMBALA 2013

ÇENGEL, Y. A.; CIMBALA, J. M.: *Fluid Mechanics Fundamentals and Applications*. 3rd. New York: McGraw-Hill Education, 2013.

CHEN ET AL. 2018

CHEN, X.; WANG, X.; CHEN, P. G.; LIU, Q.: *Determination of Diffusion Coefficient in Droplet Evaporation Experiment Using Response Surface Method*. Microgravity Science and Technology 30 (2018), pp. 675–682. DOI: 10.1007/s12217-018-9645-2.

CHORIN 1968

CHORIN, A. J.: *Numerical solution of the Navier-Stokes equations*. Mathematics of computation 22.104 (1968), pp. 745–762. DOI: 10.2307/2004575.

CHU ET AL. 2010

CHU, C.; LI, M.; CHEN, Y.; KUO, Y.: *A wind tunnel experiment on the evaporation rate of Class A evaporation pan*. Journal of Hydrology 381 (2010), pp. 221–224. DOI: 10.1016/j.jhydrol.2009.11.044.

DALTON 1802

DALTON, J.: *Experimental essays on the constitution of mixed gases; on the force of steam or vapor from water and other liquids in different temperatures, both in a torricellian vacuum and in air; on evaporation and on the expansion of gases by heat*. Memoirs of the Literary and Philosophical Society of Manchester 5 (1802), pp. 535–602.

DAMKÖHLER 2011

DAMKÖHLER, F.: *Thermal management in vehicles with electric drive system*. Porsche Engineering Magazine (2011), pp. 34–36.

DASARATHAN ET AL. 2016

DASARATHAN, D.; JILESEN, J.; CROTEAU, D.; AYALA, R.: *CFD Water Management Design for a Passenger Coach with Correlation*. SAE Technical Paper (2016). DOI: 10.4271/2016-01-8155.

DEMEL ET AL. 2019

DEMEL, D.; FELDMANN, J.; SCHÜTZ, T.; TROPEA, C.: *Simulation der Regenwasserführung für eine bessere Sicht*. ATZ - Automobiltechnische Zeitschrift 121 (2019), pp. 52–55. DOI: 10.1007/s35148-019-0144-6.

DEMEL ET AL. 2021

DEMEL, D.; SCHÜTZ, T.; KÖLZER, C.; TROPEA, C.: *Anwendungen für Mehrphasen-CFD am Fahrzeugexterieur*. Forsch Ingenieurwes 85 (2021), pp. 679–690. DOI: 10.1007/s10010-021-00480-z.

DIANAT ET AL. 2017

DIANAT, M.; SKARYSZ, M.; GARMORY, A.: *A Coupled Level Set and Volume of Fluid method for automotive exterior water management applications*. International Journal of Multiphase Flow 91 (2017), pp. 19–38. DOI: 10.1016/j.ijmultiphaseflow.2017.01.008.

DRUMM ET AL. 2008

DRUMM, C.; TIWARI, S.; KUHNERT, J.; BART, H.: *Finite pointset method for simulation of the liquid - liquid flow field in an extractor*. Computers & Chemical Engineering 32.12 (2008), pp. 2946–2957. ISSN: 0098-1354. DOI: <http://dx.doi.org/10.1016/j.compchemeng.2008.03.009>.

ESI GROUP 2024

ESI GROUP: *ESI-OpenFOAM*. <https://www.openfoam.com/about-esi-opencfd>. 2024.

FAN ET AL. 2018

FAN, C.-M.; CHU, C.-N.; SARLER, B.; LI, T.-H.: *Numerical solutions of waves-current interactions by generalized finite difference method*. Engineering Analysis with Boundary Elements 100 (2018), pp. 150–163. DOI: <https://doi.org/10.1016/j.enganabound.2018.01.010>.

FASSHAUER & ZHANG 2007

FASSHAUER, G. E.; ZHANG, J. G.: *On choosing “optimal” shape parameters for RBF approximation*. Numerical Algorithms 45 (2007), pp. 345–368. DOI: 10.1007/s11075-007-9072-8.

FITZGERALD 1886

FITZGERALD, D.: *Evaporation*. Trans. Am. Soc. Civil Eng. 98(HY12) (1886), pp. 2073–2085.

GALLERO ET AL. 2020

GALLERO, F. J. G.; MAESTRE, I.; BLÁZQUEZ, J. F.; BALADÉS, J. D. M.: *Enhanced CFD-based approach to calculate the evaporation rate in swimming pools*. Science and Technology for the Built Environment 27 (2020), pp. 524–532. DOI: 10.1080/23744731.2020.1868219.

GAVETE ET AL. 2017

GAVETE, L.; UREÑA, F.; BENITO, J.; GARCÍA, A.; UREÑA, M.; SALETE, E.: *Solving second order non-linear elliptic partial differential equations using generalized finite difference method*. Journal of Computational and Applied Mathematics 318 (2017). Computational and Mathematical Methods in Science and Engineering CMMSE-2015, pp. 378–387. ISSN: 0377-0427. DOI: <https://doi.org/10.1016/j.cam.2016.07.025>.

GERASIMOV & YURIN 2018

GERASIMOV, D. N.; YURIN, E. I.: *Kinetics of Evaporation*. 1st. Cham, Switzerland: Springer International Publishing AG, 2018.

GINGOLD & MONAGHAN 1977

GINGOLD, R. A.; MONAGHAN, J. J.: *Smoothed particle hydrodynamics: theory and application to non-spherical stars*. Monthly Notices of the Royal Astronomical Society 181 (3 1977), pp. 375–389. DOI: 10.1093/mnras/181.3.375.

GUO ET AL. 2014

GUO, Z.; FLETCHER, D.; HAYNES, B.: *A review of computational modelling of flow boiling in microchannels*. Journal of Computational Multiphase Flows 6 (2 2014), pp. 79–110. DOI: 10.1260/1757-482X.6.2.79.

HARBECK 1962

HARBECK, G.: *A practical field technique for measuring reservoir evaporation utilizing mass-transfer theory*. Geological Survey Professional Paper 272-E (1962), pp. 101–105.

HARDT & WONDRA 2008

HARDT, S.; WONDRA, F.: *Evaporation model for interfacial flows based on a continuum-field representation of the source terms*. Journal of Computational Physics 227 (11 2008), pp. 5871–5895. DOI: 10.1016/j.jcp.2008.02.020.

HICKEY ET AL. 2000

HICKEY, C.; RASPET, R.; SLATON, W.: *Effects of thermal diffusion on sound attenuation in evaporating and condensing gas-vapor mixtures in tubes*. The Journal of the Acoustical Society of America 107 (2000), p. 1126. DOI: 10.1121/1.428403.

HILBRUNNER 2005

HILBRUNNER, F.: *Ein Beitrag zur Feuchtekompensation von Präzisionsmessgeräten*. PhD thesis. Technische Universität Ilmenau, 2005.

HIRT & NICHOLS 1981

HIRT, C.; NICHOLS, B.: *Volume of fluid (VOF) method for the dynamics of free boundaries*. Journal of Computational Physics 39 (1 1981), pp. 201–225. DOI: 10.1016/0021-9991(81)90145-5.

HISATAKE ET AL. 1995

HISATAKE, K.; FUKUDA, M.; KIMURA, J.; MAEDA, M.; FUKUDA, Y.: *Experimental and theoretical study of evaporation of water in a vessel*. Journal of Applied Physics 77 (1995), p. 6664. DOI: 10.1063/1.359079.

HISATAKE ET AL. 1993

HISATAKE, K.; TANAKA, S.; AIZAWA, Y.: *Evaporation rate of water in a vessel*. Journal of Applied Physics 73 (1993), p. 7395. DOI: 10.1063/1.354031.

HOLZMANN 2017

HOLZMANN, T.: *Mathematics, Numerics, Derivations and OpenFOAM(R)*. 7th. Leoben: Holzmann CFD, 2017. URL: www.holzmann-cfd.de.

HOSSEINI ET AL. 2014

HOSSEINI, V. R.; CHEN, W.; AVAZZADEH, Z.: *Numerical solution of fractional telegraph equation by using radial basis functions*. Engineering Analysis with Boundary Elements 38 (2014), pp. 31–39. DOI: 10.1016/j.enganabound.2013.10.009.

HOSSEINI ET AL. 2022

HOSSEINI, V. R.; KOUSHKI, M.; ZOU, W. N.: *The meshless approach for solving 2D variable-order time-fractional advectiondiffusion equation arising in anomalous transport*. Engineering with Computers 38 (2022), pp. 2289–2307. DOI: 10.1007/s00366-021-01379-7.

INCROPERA ET AL. 2006

INCROPERA, F. P.; DEWITT, D. P.; BERGMAN, T. L.; LAVINE, A. S.: *Fundamentals of Heat and Mass Transfer*. 6th. New Jersey: John Wiley & Sons, 2006.

ISSA 1986

ISSA, R.: *Solution of the implicitly discretised fluid flow equations by operator-splitting*. Journal of Computational Physics 62 (1986), pp. 40–65. DOI: 10.1016/0021-9991(86)90099-9.

JASAK 1996

JASAK, H.: *Error Analysis and Estimation for the Finite Volume Method With Applications to Fluid Flows*. PhD thesis. Imperial College London, 1996.

JEFFERIES ET AL. 2015

JEFFERIES, A.; KUHNERT, J.; ASCHENBRENNER, L.; U., U. G.: *Finite Pointset Method for the Simulation of a Vehicle Travelling Through a Body of Water. Mesh-free Methods for Partial Differential Equations VII*. Ed. by M. GRIEBEL; M. A. SCHWEITZER. Springer, 2015, pp. 205–221. DOI: 10.1007/978-3-319-06898-5_11.

KALINAY 2017

KALINAY, R.: *CFD Modelling of Horizontal Water Film Evaporation*. MA thesis. Czech Technical University in Prague, 2017.

KARBON & LONGMAN 1998

KARBON, K.; LONGMAN, S.: *Automobile Exterior Water Flow Analysis Using CFD and Wind Tunnel Visualization*. SAE Technical Paper (1998). DOI: 10.4271/980035.

KISSLING ET AL. 2010

KISSLING, K.; SPRINGER, J.; JASAK, H.; SCHUTZ, S.; URBAN, K.; PIESCHE, M.; SCHÜTZ, S.; URBAN, K.; PIESCHE, M.: *A Coupled Pressure Based Solution Algorithm Based on the Volume-of-Fluid Approach for Two Or More Immisible Fluids*. V European Conference on Computational Fluid Dynamics. Lisbon, Portugal, 2010.

KONSTANTINOV 1966

KONSTANTINOV, A. R.: *Evaporation in Nature*. 1st. Leningrad: IPST, 1966.

KRAUS ET AL. 2022

KRAUS, H.; KUHNERT, J.; MEISTER, A.; SUCHDE, P.: *A Meshfree Point Collocation Method for Elliptic Interface Problems*. Applied Mathematical Modelling 113 (2022), pp. 241–261. ISSN: 0307-904X. DOI: <https://doi.org/10.1016/j.apm.2022.08.002>.

KUHNERT 2014

KUHNERT, J.: *Meshfree numerical scheme for time dependent problems in fluid and continuum mechanics*. Advances in PDE Modeling and Computation. Ed. by S. SUNDAR. ISBN: 978-93-8365-604-2. New Delhi: Ane Books, 2014, pp. 119–136. ISBN: 978-93-8365-604-2.

KUHNERT ET AL. 2017

KUHNERT, J.; MICHEL, I.; MACK, R.: *Fluid Structure Interaction (FSI) in the MESH-FREE Finite Pointset Method (FPM): Theory and Applications*. Meshfree Methods for Partial Differential Equations IX. Ed. by M. GRIEBEL; M. A. SCHWEITZER. Springer, 2017, pp. 79–92. ISBN: 978-3-030-15118-8. DOI: 10.1007/978-3-030-15119-5_5.

KUMAR ET AL. 2020

KUMAR, M.; MAURYA, S.; KUMAR, V.: *CFD Simulation of Multiphase Droplet Evaporation*. Recent Asian Research on Thermal and Fluid Sciences. Singapore: Springer Singapore, 2020, pp. 495–503. DOI: 10.1007/978-981-15-1892-8_38.

LAAROUSSI ET AL. 2008

LAAROUSSI, N.; LAURIAT, G.; DESRAYAUD, G.: *Effects of variable density for film evaporation on laminar mixed convection in a vertical channel*. International Journal of Heat and Mass Transfer 52 (2008), pp. 151–164.

LAUNDER & SPALDING 1974

LAUNDER, B.; SPALDING, D.: *The numerical computation of turbulent flows*. Computer Methods in Applied Mechanics and Engineering 3 (2 1974), pp. 269–289. DOI: 10.1016/0045-7825(74)90029-2.

LEE 2020

LEE, J.: *Evaporation Simulation on Vehicle Parts using the Thin Film Approximation*. MA thesis. Technical University of Munich (TUM), 2020.

LEE ET AL. 2022a

LEE, J.; BÄDER, D.; REHFELDT, S.; EISENTRÄGER, A.; KUHNERT, J.; MICHEL, I.; KLEIN, H.: *Two-phase MESHFREE simulations with mass transfer model for free water surface evaporation*. 15th World Congress on Computational Mechanics & 8th Asian Pacific Congress on Computational Mechanics. International Association for Computational Mechanics. July 2022.

LEE ET AL. 2022b

LEE, J.; BÄDER, D.; REHFELDT, S.; EISENTRÄGER, A.; KUHNERT, J.; MICHEL, I.; KLEIN, H.: *Two-phase water evaporation MESHFREE CFD method for wet automotive component dry-out time prediction*. SIMVEC (SIMulation in VEhiCle) 2022. VDI Wissensforum. Nov. 2022.

LEE ET AL. 2023a

LEE, J.; BÄDER, D.; REHFELDT, S.; EISENTRÄGER, A.; KUHNERT, J.; MICHEL, I.; SUCHDE, P.; KLEIN, H.: *Modeling evaporation with a meshfree collocation approach*. Computational Particle Mechanics 10 (2023), pp. 1989–2007. DOI: 10.1007/s40571-023-00602-0.

LEE ET AL. 2022c

LEE, J.; BÄDER, D.; REHFELDT, S.; KLEIN, H.: *VOF-based concentration-gradient-driven mass transfer model for water evaporation*. 10th OpenFOAM Conference. ESI Group. Nov. 2022.

LEE ET AL. 2023b

LEE, J.; BÄDER, D.; REHFELDT, S.; KLEIN, H.: *Dry-Out Time Prediction of Automotive Applications with Water Evaporation CFD using a Meshfree Collocation Approach*. NAFEMS International Multiphysics Conference. NAFEMS. Nov. 2023.

LEE ET AL. 2023c

LEE, J.; BÄDER, D.; REHFELDT, S.; KLEIN, H.: *Water Evaporation CFD Method with a Meshfree Collocation Approach for Wet Automotive Component Dry-out time Prediction*. JSAE Autumn 2023. Society of Automotive Engineers of Japan. Oct. 2023.

LEE ET AL. 2024

LEE, J.; BÄDER, D.; REHFELDT, S.; KLEIN, H.: *Water Evaporation CFD Method with the Meshfree Volume-Volume-Coupling Approach for Wet Automotive Component Dry-Out Time Prediction*. International Journal of Automotive Engineering 15.1 (2024), pp. 58–65. DOI: 10.20485/jsaeijae.15.1_58.

LI & HEISELBERG 2005

LI, Z.; HEISELBERG, P.: *CFD Simulations for Water Evaporation and Airflow Movement in Swimming Baths*. Aalborg Universitet, 2005.

LISZKA & ORKISZ 1980

LISZKA, T.; ORKISZ, J.: *The finite difference method at arbitrary irregular grids and its application in applied mechanics*. Computers & Structures 11 (1980), pp. 83–95. DOI: 10.1016/0045-7949(80)90149-2.

LIU & LIU. 2003

LIU, G. -R.; LIU., M. B.: *Smoothed particle hydrodynamics: a meshfree particle method*. Singapore: World Scientific, 2003.

LÖHNER & OÑATE 2004

LÖHNER, R.; OÑATE, E.: *A general advancing front technique for filling space with arbitrary objects*. International Journal for Numerical Methods in Engineering 61 (2004), pp. 1977–1991. DOI: 10.1002/nme.1068.

MAI-DUY & TRAN-CONG 2001

MAI-DUY, N.; TRAN-CONG, T.: *Numerical solution of NavierStokes equations using multiquadric radial basis function networks*. International Journal for Numerical Methods in Fluids 37 (2001), pp. 65–86. DOI: 10.1002/flid.165.

MAKANA ET AL. 2016

MAKANA, M.; KUMAR, G.; REGIN, F.: *Passenger Car Water Wading Evaluation Using CFD Simulation*. SAE Technical Paper (2016). DOI: 10.4271/2016-28-0072.

MASONER ET AL. 2008

MASONER, J.; STANNARD, D.; CHRISTENSON, S.: *Differences in Evaporation Between a Floating Pan and Class A Pan on Land*. JAWRA Journal of the American Water Resources Association 44 (2008), pp. 552–561. DOI: 10.1111/j.1752-1688.2008.00181.x.

MEREDITH ET AL. 2011

MEREDITH, K. V.; XIN, Y.; VRIES, J.: *A Numerical Model for Simulation of Thin-Film Water Transport over Solid Fuel Surfaces*. Fire Safety Science 10 (2011), pp. 415–428. DOI: 10.3801/IAFFS.FSS.10-415.

MESHFREE TEAM 2023

MESHFREE TEAM: *MESHFREE [software]*. Fraunhofer ITWM & SCAI. Germany, 2023. URL: <https://www.meshfree.eu/>.

MEYER 1915

MEYER, A. F.: *Computing Run-Off from rainfall and other physical data*. Trans. Am. Soc. Civil Eng. 79 (1915), pp. 1055–1155.

MICHEL ET AL. 2021

MICHEL, I.; SEIFARTH, T.; KUHNERT, J.; SUCHDE, P.: *A meshfree generalized finite difference method for solution mining processes*. Computational Particle Mechanics 8 (2021), pp. 561–574. DOI: 10.1007/s40571-020-00353-2.

MOLTRECHT 2016

MOLTRECHT, L.: *Direct Numerical Simulation of Droplet Evaporation in OpenFOAM*. MA thesis. RWTH Aachen University, 2016.

MONGILLO 2011

MONGILLO, M.: *Choosing Basis Functions and Shape Parameters for Radial Basis Function Methods*. SIAM Undergraduate Research Online 4 (2011), pp. 190–209. DOI: 10.1137/11S010840.

MORTON 1968

MORTON, F. I.: *Evaporation and climate: A study in cause and effect*. PhD thesis. Trinity College, University of Dublin, 1968.

MOUKALLED ET AL. 2016

MOUKALLED, F.; MANGANI, L.; DARWISH, M.: *The Finite Volume Method in Computational Fluid Dynamics*. 1st. Switzerland: Springer Cham, 2016. ISBN: 978-3-319-16873-9. DOI: 10.1007/978-3-319-16874-6_1.

PATANKAR 1980

PATANKAR, S.: *Numerical Heat Transfer and Fluid Flow*. 1st. Boca Raton: CRC Press, 1980. DOI: 10.1201/9781482234213.

POPOV 2015

POPOV, B. N.: *Corrosion Engineering: Principles and Solved Problems*. Amsterdam: Elsevier B.V., 2015.

RAGAB & WANG 2012

RAGAB, R.; WANG, T.: *An Investigation of Liquid Droplet Evaporation Model Used in Multiphase Flow Simulation*. 2012, pp. 485–497. DOI: 10.1115/IMECE2012-87392.

RATTNER & GARIMELLA 2018

RATTNER, A. S.; GARIMELLA, S.: *Simulation of Taylor flow evaporation for bubble-pump applications*. International Journal of Heat and Mass Transfer 116 (2018), pp. 231–247. DOI: j.ijheatmasstransfer.2017.08.110.

REVIE 2015

REVIE, R. W.: *Corrosion and Corrosion Control: An Introduction to Corrosion Science and Engineering*. 4th. Hoboken, New Jersey: John Wiley & Sons, Inc., 2015.

ROBERGE 2008

ROBERGE, P. R.: *Corrosion Engineering: Principles And Practice*. New York: Mcgraw-hill Companies, 2008.

ROHWER 1931

ROHWER, C.: *Evaporation from free water surfaces*. US Department of Agriculture, Washington, D.C. Technical Bulletin 271 (1931).

SARLER 2005

SARLER, B.: *A Radial Basis Function Collocation Approach in Computational Fluid Dynamics*. Computer Modeling in Engineering & Sciences 7.2 (2005), pp. 185–194. DOI: 10.3970/cmcs.2005.007.185.

SAUFI ET AL. 2019

SAUFI, A.; FRASSOLDATI, A.; FARAVELLI, T.; CUOCI, A.: *DropletSMOKE++: A comprehensive multiphase CFD framework for the evaporation of multidimensional fuel droplets*. International Journal of Heat and Mass Transfer 131 (2019), pp. 836–853. DOI: 10.1016/j.ijheatmasstransfer.2018.11.054.

SCHASCHKE 2014

SCHASCHKE, C.: *A Dictionary of Chemical Engineering*. 1st. Oxford University Press, 2014.

SCHLOTTKE & WEIGAND 2008

SCHLOTTKE, J.; WEIGAND, B.: *Direct numerical simulation of evaporating droplets*. Journal of Computational Physics 227 (10 2008), pp. 5215–5237. DOI: doi.org/10.1016/j.jcp.2008.01.042.

SCHWEITZER 2004

SCHWEITZER, P. A.: *Encyclopedia of Corrosion Technology*. 2nd. New York: Marcel Dekker, 2004.

SEIFARTH 2018

SEIFARTH, T.: *Numerische Algorithmen für Gitterfreie Methoden zur Lösung von Transportproblemen*. PhD thesis. Germany: Universität Kassel, 2018.

SINGH & XU 1997a

SINGH, V.; XU, C.-Y.: *Evaluation and generalization of 13 mass-transfer equations for determining free water evaporation*. Hydrological Processes 11 (1997), pp. 311–323.

SINGH & XU 1997b

SINGH, V.; XU, C.-Y.: *Sensitivity of Mass Transfer-Based Evaporation Equations to Errors in Daily and Monthly Input Data*. Hydrological Processes 11 (1997), pp. 1465–1473.

SINGH & XU 1998

SINGH, V.; XU, C.-Y.: *Evaluation and generalization of 13 mass-transfer equations for determining free water evaporation*. Hydrological Processes 11.3 (1998), pp. 311–323. DOI: 10.1002/(SICI)1099-1085(19970315)11:3<311::AID-HYP446>3.0.CO;2-Y.

SOH ET AL. 2016

SOH, G. Y.; YEOH, G. H.; TIMCHENKO, V.: *An algorithm to calculate interfacial area for multiphase mass transfer through the volume-of-fluid method*. International Journal of Heat and Mass Transfer 100 (2016), pp. 573–581. DOI: 10.1016/j.ijheatmasstransfer.2016.05.006.

SOSNOWSKI ET AL. 2013

SOSNOWSKI, P.; PETRONIO, A.; ARMENIO, V.: *Numerical model for thin liquid film with evaporation and condensation on solid surfaces in systems with conjugated heat transfer*. International Journal of Heat and Mass Transfer 66 (2013), pp. 382–395. DOI: 10.1016/j.ijheatmasstransfer.2013.07.045.

STANHILL 2002

STANHILL, G.: *Is the Class-A evaporation pan still the most practical and accurate meteorological method for determining irrigation water requirements?*: Agricultural and Forest Meteorology 112 (2002), pp. 233–236. DOI: 10.1016/S0168-1923(02)00132-6.

SUBRAMANYA 2008

SUBRAMANYA, K.: *Engineering Hydrology*. 3rd. New Delhi, India: Tata McGraw-Hill Publishing Company Limited, 2008.

SUCHDE 2018

SUCHDE, P.: *Conservation and Accuracy in Meshfree Generalized Finite Difference Methods*. PhD thesis. Germany: University of Kaiserslautern, 2018.

SUCHDE ET AL. 2017

SUCHDE, P.; KUHNERT, J.; SCHRÖDER, S.; KLAR, A.: *A flux conserving meshfree method for conservation laws*. International Journal for Numerical Methods in Engineering 112.3 (2017), pp. 238–256. DOI: 10.1002/nme.5511.

SUCHDE ET AL. 2018

SUCHDE, P.; KUHNERT, J.; TIWARI, S.: *On meshfree GFDM solvers for the incompressible Navier–Stokes equations*. Computers & Fluids 165 (2018), pp. 1–12. DOI: 10.1016/j.compfluid.2018.01.008.

SUCHDE ET AL. 2023

SUCHDE, P.; LEITHÄUSER, C.; KUHNERT, J.; BORDAS, S. P.: *Volume and Mass Conservation in Lagrangian Meshfree Methods*. arXiv Physics Fluid Dynamics (2023). DOI: 10.48550/arXiv.2303.13410.

SUCHDE ET AL. 2022

SUCHDE, P.; JACQUEMIN, T.; DAVYDOV, O.: *Point Cloud Generation for Meshfree Methods: An Overview*. Archives of Computational Methods in Engineering 30 (2022), pp. 1–27. DOI: <https://doi.org/10.1007/s11831-022-09820-w>.

SUCHDE & KUHNERT 2018

SUCHDE, P.; KUHNERT, J.: *Point cloud movement for fully Lagrangian meshfree methods*. Journal of Computational and Applied Mathematics 340 (2018), pp. 89–100. DOI: 10.1016/j.cam.2018.02.020.

VAN DER VORST 1992

VAN DER VORST, H. A.: *Bi-CGSTAB: A fast and smoothly converging variant of Bi-CG for the solution of nonsymmetric linear systems*. SIAM Journal on scientific and Statistical Computing 13.2 (1992), pp. 631–644. DOI: 10.1137/0913035.

VARSHNEY ET AL. 2021

VARSHNEY, M.; PASUNURTHI, S.; MAITI, D.; SRINIVASAN, C.: *CFD Method Development for Simulating Water Fording for a Passenger Car*. SAE Technical Paper (2021). DOI: 10.4271/2021-01-0205.

VERSTEEG & MALALASEKERA 2007

VERSTEEG, H. K.; MALALASEKERA, W.: *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*. 2nd. New York: McGraw-Hill Education, 2007.

VIDAL-LÓPEZ ET AL. 2012

VIDAL-LÓPEZ, P.; MARTIN-GORRIZ, B.; MARTÍNEZ-ALVAREZ, V.; GALLEGO-ELVIRA, B.: *CFD simulation of water evaporation in Class-A pan with a transient analysis*. Acta Horticulturae 1008 (2012), pp. 91–96. DOI: 10.17660/ActaHortic.2013.1008.11.

WANG ET AL. 2020

WANG, D.; QIANG, H.; SHI, C.: *A multiphase SPH framework for solving the evaporation and combustion process of droplets*. International Journal of Numerical Methods for Heat and Fluid Flow 30 (3 2020), pp. 1547–1575. DOI: 10.1108/HFF-08-2019-0666.

WICKERT ET AL. 2020

WICKERT, D.; HERMSDORF, F.; PROKOP, G.: *Analysis of the Water Management on a Full Virtual Car Using Computational Fluid Dynamics*. SAE Int. J. Mater. Manf. 13.2 (2020), pp. 175–191. DOI: 10.4271/05-13-02-0013.

WICKERT & PROKOP 2021

WICKERT, D.; PROKOP, G.: *Simulation of water evaporation under natural conditions - a state-of-the-art overview*. Experimental and Computational Multiphase Flow 3 (2021), pp. 242–249. DOI: 10.1007/s42757-020-0071-5.

YANG & KONG 2017

YANG, X.; KONG, S. C.: *Smoothed particle hydrodynamics method for evaporating multiphase flows*. Phys. Rev. E 96.3 (2017), p. 033309. DOI: 10.1103/PhysRevE.96.033309.