Numerical Simulation of the Dynamics of Vortex Cavitation

Faraz Khatami

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with Application to Ship Propellers and Pump Impellers

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NUMERICAL SIMULATION OF THE DYNAMICS OF VORTEX CAVITATION

WITH APPLICATION TO SHIP PROPELLERS AND PUMP IMPELLERS

PROEFSCHRIFT

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SUMMARY

A computational framework has been developed for numerical simulation of cavitating flows, in particular flows with cavitating vortices. The computational approach is based on the URANS equations for compressible turbulent flow, as well as the Euler equations for compressible inviscid flow. The equilibrium cavitation model of Saurel, Schnerr, and Schmidt is employed. This single-fluid model assumes local thermodynamic and mechanical equilibrium in the mixture region of the flow. The main contributions of the present thesis are the following.

It was found that for a computational method that directly uses the thermodynamic closure relations, more than 90% of the computational time is spent in computations associated with these relations. To circumvent this problem, this computationally costly method is replaced by using precomputed 2D multiphase thermodynamic tables in the $\rho - e$ plane, with density ρ , and internal energy e . The tables provide the required primitive variables, which include pressure, speed of sound, temperature, and vapor void fraction, with no need to determine the flow phase. The thermodynamic computations using this approach do not require much computational effort. The main difficulty in preparing these multiphase tables is due to the slope discontinuities in the phase-transitioning regions near the saturation curves. In these regions, the conventional look-up approaches are inaccurate and inefficient since their accuracy is insensitive to data grid refinements. To remove this bottleneck, a novel interpolation approach, named POITC, has been developed. The POITC method is fast, and, compared to the conventional interpolation methods, the POITC interpolation approach is uniformly accurate in the whole $(\rho - e)$ plane specifically near the saturation curves. It is several orders of magnitude more accurate than the conventional interpolation methods. This technique allows for preparing very efficient (small size of underlying data) multiphase tables.

One of the main numerical difficulties of numerical simulations of compressible flows with cavitation is due to strong discontinuities and sharp gradients occurring at the captured interfaces of the fluid phases as well as near shock waves. For example, for water at standard conditions, the density ratio of liquid to vapor is $\frac{\rho_l}{\rho_v} = 58,000$. For truly resolving the discontinuities in the flow field, impractically fine grid resolutions are required.

Alternatively, shock capturing schemes, such as the MUSCL family of schemes, can be employed, which use artificial dissipation in order to capture the discontinuities in the flow fields. The artificial dissipation is needed for stable numerical simulations of cavitating flows. However, in the case of turbulent cavitating flow, the artificial dissipation is highly undesirable. To remedy this problem, extremely fine resolution of the computational grid

is required for these schemes. Moreover, it is shown that, to resolve the physics of the problem and in order to satisfy the condition of numerical stability, the allowed time steps are extremely small (order of nano seconds). Therefore, the need for extremely fine grids in combination with very small time steps render the usage of the MUSCL schemes for efficient and accurate numerical simulations of turbulent cavitating flows impractical, i.e. the case of the turbulent flow with cavitating vortices in the present thesis.

To improve the accuracy and efficiency of the spatial discretizations, the higher-order accurate WENO schemes are considered. The WENO scheme is a very low-dissipative scheme, i.e. it has an almost negligible amount of numerical dissipation, and it is thus a well-suited candidate scheme for the numerical simulations of the compressible turbulent flows with cavitation. However, the WENO scheme is not strictly monotonic, which can result in non-physical solutions near sharp gradients and discontinuities in the flow field variables. In order to avoid such problems, the scheme must obey a positivity principle or a maximum principle. The maximum principle-preserving SL-WENO scheme from literature is employed. Additionally, a novel low-dissipative limiter-free (no slope/flux limiters) positivity-preserving strategy has been developed for the WENO scheme. This new scheme, named log-WENO, uses the properties of logarithmic and exponential transformations in order to satisfy the positivity-preserving property of the numerical solution. The log-WENO scheme is relatively simple, and computationally low-cost.

In order to assess its performance and accuracy, the developed numerical framework has been applied to several test cases. It is then employed for the numerical simulation of a number of principal test cases. The MUSCL scheme in combination with the POITC method has been applied to the numerical simulations of cavitating expanding waves in 1D space, the flow around a 2D NACA0015 hydrofoil with sheet cavitation, and tip vortex cavitation in the flow around Arndt's 3D elliptic hydrofoil. Additionally, the conventional higher-order accurate multidimensional WENO reconstruction scheme, in combination with the POITC method, has been applied to the numerical simulations of cavitating flows, in which the discontinuities are not very strong (no need to obey the maximum principle), in particular for cavitating flow around the 2D NACA0015 hydrofoil. Finally, numerical simulations of cavitating expanding waves in 1D space are performed employing the POITC approach, and using higher-order accurate schemes, which include the maximum principle-preserving SL-WENO scheme, as well as the developed positivity-preserving log-WENO scheme.

SAMENVATTING

Dit proefschrift beschrijft de ontwikkeling van een rekenmethode voor de numerieke simulatie van caverende stromingen, in het bijzonder stromingen met caverende wervels. De rekenmethode is gebaseerd op de instationaire Reynolds-gemiddelde Navier-Stokes (URANS) vergelijkingen voor samendrukbare turbulente stromingen, of op de Euler vergelijkingen voor samendrukbare niet-viskeuze stromingen. In de rekenmethode wordt gebruik gemaakt van het evenwichts-cavitatie model van Saurel, Schnerr en Schmidt. In dit model wordt mechanisch en thermodynamisch evenwicht aangenomen tussen de twee fasen van het twee-fasen fluïdum, dat daardoor als een enkelvoudig fluïdum kan worden gemodelleerd, met thermodynamische sluitingsrelaties voor de vloeistof, voor de damp en voor het vloeistof-damp mengsel. De belangrijkste bijdragen van het proefschrift zijn hieronder samengevat.

Voor een rekenmethode waarin de uitdrukkingen voor de thermodynamische sluitingsrelaties rechtstreeks zijn geïmplementeerd is geconstateerd dat meer dan 90% van de rekentijd wordt besteed aan het berekenen van deze relaties. Dat leidt tot extreem lange rekentijden. Dit probleem kan worden vermeden door gebruik te maken van vooraf berekende tabellen waarmee de thermodynamische grootheden als functie van dichtheid ρ en interne energie e worden bepaald. De tabellen leveren de in de rekenmethode benodigde primitieve variabelen als druk, temperatuur en dampfractie, zowel als de geluidssnelheid, zonder dat daarvoor de fase van het fluïdum bekend hoeft te zijn.

Door gebruik te maken van de tabellen vergen de thermodynamische berekeningen nog slechts een geringe rekeninspanning. Dat leidt tot een substantiële reductie van de rekentijd van de rekenmethode. De belangrijkste moeilijkheid bij het opstellen van de thermodynamische tabellen zijn de gebieden in het (ρ, e) -vlak waar de faseovergang plaats vindt, dus ter plaatse van de verzadigingskrommes. Ter plaatse van de verzadigingskrommes bevinden zich discontinuïteiten in de afgeleiden van de thermodynamische grootheden als functie van dichtheid en interne energie. In het gebied in de buurt van de verzadigingskrommes is de conventionele interpolatie methode in de tabelopzoekprocedure onnauwkeurig en inefficiënt. De reden is dat verfijning van het rechthoekige netwerk waarop de data vooraf is berekend vanwege de discontinuïteiten niet leidt tot grotere nauwkeurigheid in dat gebied. Dit probleem is opgelost door het ontwikkelen en implementeren van een nieuwe interpolatie methode, de Phase-Oriented Interpolation in Transition Cells (POITC) genaamd. De POITC methode is snel en, in tegenstelling tot de conventionele interpolatiemethode, is de POITC interpolatiemethode uniform nauwkeurig in het hele (ρ, e) -vlak, met name ook nabij de verzadigingskrommes. Daardoor is de nieuwe methode meerdere ordes nauwkeuriger dan de conventionele interpolatiemethode.

Met behoud van nauwkeurigheid kunnen de onderliggende tabellen voor de POITC interpolatiemethode aanzienlijk beperkter van omvang zijn, waardoor ten opzichte van de conventionele interpolatiemethode de benodigde omvang van het geheugen is gereduceerd.

Bij de numerieke simulatie van samendrukbare stromingen met cavitatie vormt het optreden van discontinuïteiten, sterke schokken en fasescheidingsoppervlakken, een uitdaging voor gebruikelijke numerieke schema's. Bijvoorbeeld, de verhouding van de dichtheid van water en die van waterdamp is bij standaard condities gelijk aan $\frac{\rho_l}{\rho_v} = 58,000$. Om in de numerieke oplossing deze discontinuïteiten, vaak met een complexe topologie, daadwerkelijk te representeren zouden rekennetwerken noodzakelijk zijn met een, niet-praktische, extreem hoge resolutie.

Voor dit soort stromingen bieden numerieke schema's zoals de familie van MUSCL schema's, een alternatief. Deze schema's introduceren artificiële dissipatie waardoor de discontinuïteiten worden uitgesmeerd tot gebieden met een sterke gradiënt in de numerieke oplossing. De artificiële dissipatie is noodzakelijk voor de numerieke stabiliteit van de numerieke simulatie van caverende stromingen. Echter, in het geval van turbulente caverende wervelstromingen is artificiële dissipatie ongewenst. De remedie voor dit probleem is, weer, het gebruiken van rekennetwerken met extreem hoge resolutie. Bovendien is bekend dat voor de resolutie van de fysische stromingsfenomenen en voor het voldoen aan de numerieke stabiliteitsconditie, de toegestane tijdstap extreem klein moet zijn, orde van nanoseconden. De noodzaak van extreem fijne rekennetwerken in combinatie met een erg kleine tijdstap, maakt dat het gebruik van MUSCL schema's voor een efficiënte en nauwkeurige numerieke simulatie van turbulente caverende stromingen, in dit proefschrift turbulente stroming met caverende wervels, niet praktisch is.

Om de nauwkeurigheid en efficiëntie van de ruimtelijke discretisatie te verbeteren is de toepassing van hogere-orde WENO schema's bestudeerd. Het WENO schema is een numeriek schema met een vrijwel verwaarloosbare hoeveelheid numerieke dissipatie. Daarom is het een geschikt kandidaat schema voor een rekenmethode voor de numerieke simulatie van compressibele turbulente stromingen met cavitatie. Wel is het WENO schema niet strikt monotoon, mogelijkwerwijze resulterend in niet-fysische oplossingen nabij scherpe gradienten en discontinuïteiten in de stromingsveld grootheden. Om deze problemen te vermijden moet het schema voldoen aan het positiviteit principe of aan het maximum principe. Hier wordt gebruik gemaakt van het uit de literatuur bekende SL-WENO schema dat aan het maximum-principe voldoet. Voor dit WENO schema is een nieuw laag-dissipatief, positiviteit-behoudende strategie ontwikkeld waarvoor geen ("slope/flux") begrenzers nodig zijn. Dit nieuwe schema, het zogenaamde log-WENO schema, maakt gebruik van de eigenschappen van logaritmische en exponentiele transformaties die de positiviteit-behoudende eigenschap van de numerieke oplossing waarborgen. Het log-WENO schema is een relatief eenvoudig schema dat weinig rekeninspanning vergt.

De prestatie en de nauwkeurigheid van de rekenmethode gebaseerd op verschillende schema's zijn geanalyseerd aan de hand van toepassing van de rekenmethode op een aantal testgevallen. De rekenmethode met het MUSCL schema, in combinatie met de POITC interpolatiemethode, is toegepast op het test geval van de 1D expanderende caverende stroming in een buis, de stroming om een 2D NACA0015 hydrofoil met vliescavitatie en de stroming om Arndt's 3D hydrofoil met elliptische planform. In het laatste test geval treedt tipwervel cavitatie op. Verder is de rekenmethode met het conventionele hogere-orde meer-dimensionale WENO reconstructie schema, in combinatie met de POITC interpolatie methode, toegepast op de numerieke simulatie van de caverende stroming om het 2D

NACA0015 hydrofoil. In deze stroming zijn de optredende discontinuïteiten relatief mild, zodat het niet nodig is dat het schema aan het maximum principe voldoet. Tenslotte is de rekenmethode met hogere-orde nauwkeurige schema's, inclusief het SL-WENO schema dat aan het maximum principe voldoet, zowel als het log-WENO schema dat positiviteit behoudend is, in combinatie met de POITC interpolatiemethode, met succes toegepast op de caverende expanderende stroming in een buis. In dat test geval treden sterke discontinuïteiten en scherpe gradienten op.

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NOMENCLATURE

Acronyms

Symbol	Description	Units
AOA	angle of attack	
AR	Aspect Ratio	
AUSM	Advection Upstream Splitting Method	
CFL	Courant-Friedrichs-Lewy	
Cs	Characteristic	
deg	degree	
HLLC	Harten-Lax-van Leer	
JST	Jameson-Schmidt-Turkel	
log	logarithm	
max	maximum	
min	minimum	
MUSCL	Monotonic Upstream-Centered Scheme for Conservation Laws	
NS	Navier Stokes	
POITC	Phase-Oriented Interpolations in Transition Cells	
RANS	Reynolds Averaged Navier Stokes	
S-A	Spalart-Allmaras	
SST	Shear Stress Transport	
TVD	Total Variation Diminishing	
WENO	Weighted Essentially Non-Oscillatory	

Greek Symbols

Symbol	Description	Units
α	vapor void fraction	-
$\eta = \frac{\rho}{\rho_\eta}$	nondimensional density	-
γ	specific heat ratio	-
γ_{pl}	specific heat ratio, liquid	-
γ_{pm}	specific heat ratio, mixture	-
γ_{pv}	specific heat ratio, vapor	-
$\hat{\mu}$	turbulent (eddy) viscosity	$\text{kg m}^{-1} \text{s}^{-1}$
κ	heat conductivity	$\text{W K}^{-1} \text{m}^{-1}$
μ	molecular (dynamic) viscosity	$\text{kg m}^{-1} \text{s}^{-1}$
μ_{tot}	total viscosity	$\text{kg m}^{-1} \text{s}^{-1}$
ν	laminar kinematic viscosity	$\text{m}^2 \text{s}^{-1}$
Ω_{ij}	component of vorticity tensor	s^{-1}
Ψ	a dependent thermodynamic variable	
ψ	an independent thermodynamic variable	
ρ	density	kg m^{-3}
$\rho_\eta = 1100$	reference density in simulations	kg m^{-3}
τ	pseudo time in dual time stepping method	s
τ_w	wall shear stress	Pa
$\xi = \frac{1}{c^2}$	mapped speed of sound	$\text{m}^{-2} \text{s}^2$
$\zeta = \frac{e}{e_\zeta}$	nondimensional internal energy	-
λ	eigenvalue	
$\sigma = \frac{p_\infty - p_v}{1/2 \rho_\infty U_\infty^2}$	cavitation number	-
$\tilde{\omega}$	fluid vorticity vector	s^{-1}
$\underline{\underline{\Lambda}}$	matrix of diagonal eigenvalues	

Roman Symbols

Symbol	Description	Units
β_r	smoothness indicator coefficients, WENO scheme	

$\mathcal{R}^c$	matrix of convective spatial residuals	
$\mathcal{R}^v$	matrix of viscous spatial residuals	
$\mathcal{R}$	matrix of total spatial residuals	
$\hat{\omega}$	specific turbulent dissipation	s^{-1}
$\hat{k}$	turbulent kinetic energy	J kg^{-1}
$\hat{P}_r$	turbulent Prandtl number	-
$\mathcal{C}$	CFL number	-
$\mathcal{V}$	Volume of grid cell	m^3
$\mathbf{H}$	vector of multidimensional inviscid numerical fluxes	
$\mathbf{H}^c$	vector of multidimensional convective numerical fluxes	
$\mathbf{H}^p$	vector of multidimensional pressure numerical fluxes	
$\mathbf{H}^v$	vector of multidimensional viscous numerical fluxes	
$\mathbf{n}$	normal vector	
$\tilde{E}$	relative error	-
$\underline{\underline{I}}$	identity matrix	
$\vec{\mathbf{F}}$	vector of inviscid fluxes	
$\vec{\mathbf{F}}^v$	vector of viscous fluxes	
c	speed of sound	m s^{-1}
$C_f = \frac{ \tau_w }{\frac{1}{2}\rho_\infty U_\infty^2}$	skin friction coefficient	-
c_v	specific heat at constant volume	$\text{J kg}^{-1} \text{K}^{-1}$
C_{pl}	specific heat at constant pressure, liquid	$\text{J kg}^{-1} \text{K}^{-1}$
C_{pm}	specific heat at constant pressure, mixture	$\text{J kg}^{-1} \text{K}^{-1}$
C_{pv}	specific heat at constant pressure, vapor	$\text{J kg}^{-1} \text{K}^{-1}$
c_{rj}	polynomial coefficients, WENO scheme	-
C_{vl}	specific heat at constant volume, liquid	$\text{J kg}^{-1} \text{K}^{-1}$
C_{vv}	specific heat at constant volume, vapor	$\text{J kg}^{-1} \text{K}^{-1}$
d_r	ideal weights, WENO scheme	-
E	total specific energy	J kg^{-1}
e	specific internal energy	J kg^{-1}

$e_\zeta = 2.48433698 \times 10^6$	reference internal energy in simulations	J kg^{-1}
f	frequency	Hz
f_v	mass fraction of vapor	-
F_Y	lift force	N
H	total specific enthalpy	J kg^{-1}
h	specific enthalpy	J kg^{-1}
k	index of grid cells	
K_0	constant, modified Tait equation	Pa
l	chord length of hydrofoil	m
l_s	span-wise length of hydrofoil	m
L_v	latent heat of vaporization	J kg^{-1}
m	degree of a polynomial	
$M = \frac{u}{c}$	Mach number	-
M_{co}	cut-off Mach number	-
N	constant, modified Tait equation	-
p	pressure	Pa
p_∞	free-stream pressure	Pa
p_c	critical pressure	Pa
Pr	dynamic Prandtl number	-
Q	quantity from Q-criterion	s^{-2}
R	specific gas constant	$\text{J kg}^{-1} \text{K}^{-1}$
S_{ij}	component of rate-of-strain tensor	s^{-1}
T	temperature	K
t	time	s
T_0	reference temperature	K
T_c	critical temperature	K
T_r	triple point temperature	K
u	velocity, 1D	m s^{-1}
$u_* = \sqrt{\frac{ \tau_w }{\rho}}$	friction velocity	m s^{-1}

U_∞	free-stream velocity	m s^{-1}
u_i	velocity component, $i = \{1, \dots, 3\}$	m s^{-1}
$v = \frac{1}{\rho}$	specific volume	$\text{kg}^{-1} \text{m}^3$
$V_{\text{tot}} = \frac{1}{l^3} \iiint_{\mathcal{V}} \alpha d\mathcal{V}$	3D nondimensional total vapor volume	-
w_r	nonlinear weights, WENO scheme	-
$y^+ = \frac{u_* y}{\nu}$	dimensionless wall distance	-
$\mathbf{f}$	vector of inviscid fluxes, 1D	
$\mathbf{q}$	vector of conservative variables, 1D	
$\mathbf{U}$	vector of conservative variables	
$\mathbf{n}$	normalized vector of a grid cell face	
$\mathbf{S}$	vector of a cell face	
$\mathbf{x}$	position vector	
$\text{Re}_\infty = \frac{\rho_\infty U_\infty l}{\mu_\infty}$	free-stream Reynolds number	-
$\underline{\underline{A}}$	Jacobian matrix, inviscid flux	
$\underline{\underline{M}}_{\text{conn}}$	connectivity matrix, transition cell	
$\underline{\underline{R}}^{-1}$	Matrix of left eigenvectors	
$\underline{\underline{R}}$	Matrix of right eigenvectors	
$C_p = \frac{p - p_\infty}{1/2 \rho_\infty U_\infty^2}$	pressure coefficient	-

Superscripts

Symbol	Description	Units
max	maximum	
min	minimum	
sat	saturation	
v	vapor	

Subscripts

Symbol	Description	Units
l	liquid	
m	mixture	

<i>max</i>	maximum
<i>min</i>	minimum
<i>mix</i>	mixture
<i>ref</i>	reference
<i>sat</i>	saturation
<i>v</i>	vapor

INTRODUCTION

1.1 Cavitation

Cavitation is an unsteady process of appearance and disappearance of vapor cavities. The vapor cavities form in low pressure zones of the cavitating flow field and subsequently disappear in areas where the pressure rises. In most practical situations, cavitation can and typically does start when the local static pressure of a liquid drops below its saturation pressure. Therefore, the pressure decrease in the flow field can be identified as the major driving mechanism for phase change in cavitation. This is in contrast to the boiling process in which bubbles start to appear by increasing the temperature of the liquid to its saturation temperature, i.e. increasing the temperature is the major phase change mechanism in boiling. In Figure 1.1 the cavitation and boiling processes of water are shown schematically. It is assumed that, initially there is water at standard conditions, i.e. a thermodynamic state $(T, p)_0$. When the temperature of water is increased, at constant pressure, to saturation temperature $(T'', p'')_{sat}$ boiling occurs. By decreasing the water pressure from the standard condition, at constant temperature (isothermally), to the saturation pressure $(T, p)_{sat}$, cavitation starts.

The processes shown in Figure 1.1 are only approximations of the actual case. In particular, it is assumed that for cavitation the phase change process occurs in a thermo-

Figure 1.1: Diagram of pressure vs. temperature, showing equilibrium ($T = \text{constant}$) cavitation and equilibrium boiling ($p = \text{constant}$) processes.

(a) Cavitation erosion

(b) Shock wave lithotripsy

Figure 1.2: Cavitation in practical problems: (a) an eroded surface of a ship propeller caused by cavitation [137]. (b) schematic of a shock wave lithotripsy process, which uses cavitation effects to break kidney stones [42].

dynamic equilibrium, i.e. no heat transfer between the phases. In reality the phase change occurs non-isothermally (the dotted path from $(T, p)_0$ to $(T', p')_{sat}$ in Figure 1.1), which requires heat transfer to the surrounding liquid. This process can only be accomplished in a non-equilibrium thermodynamic state. In this thesis the effect of these non-equilibrium thermodynamic processes are assumed to be negligible, and the equilibrium assumption is thus considered to be sufficient for approximating the real problem.

Cavitating flows are present in many applications: in technical applications such as pumps, turbines, ship propellers, fuel injection systems, and bearings, and in medical sciences such as in lithotripsy treatment and the flow through artificial heart valves. Cavitation may cause a number of problems in hydraulic systems. These include vibration, noise, and surface erosion in the case of developed cavitation, and deteriorating the performance of the system such as a lift reduction and an increase in drag of a hydrofoil and loss of turbomachinery efficiency. For example, Figure 1.2a shows an eroded surface of a ship propeller caused by cavitation. However, besides the undesirable effects, cavitation is used in some industrial processes to produce high-pressure peaks and apply them for cleaning of surfaces, dispersion of particles in a liquid, production of emulsions, etc and in medical applications such as shock wave lithotripsy for breaking kidney stones (see Figure 1.2b), and so on. In any case, to control its effects in widespread applications, it is vital to understand the structure and mechanisms of the cavitation phenomenon.

Following the scaling law, cavitating flows are characterized by the cavitation number σ , which is a dimensionless number defined by

$$\sigma = \frac{p_\infty - p_v}{\frac{1}{2}\rho_\infty U_\infty^2}. \quad (1.1)$$

Here, p_∞ , ρ_∞ , and U_∞ are the free-stream pressure, density, and velocity, respectively, and p_v is the vapor pressure at the bulk temperature. When the pressure, p , in the flow

is decreased, such that the minimum pressure, becomes equal to the vapor pressure p_v , cavitation is triggered. Cavitation inception, denoted by σ_i , occurs when the following relation is satisfied

$$\sigma_i = -\min(C_p), \quad (1.2)$$

where, C_p is the pressure coefficient:

$$C_p = \frac{p - p_\infty}{\frac{1}{2}\rho_\infty U_\infty^2}. \quad (1.3)$$

In this thesis, we use the condition in equation (1.2) as the cavitation inception criteria for the numerical simulations of cavitation.

However, cavitation inception is not adequately described by just the parameter σ_i in equation (1.2). In general, the cavitation threshold σ_i depends on various parameters such as flow geometry, viscosity, turbulence levels, the gas content of the liquid in terms of dissolved and free gases, etc (see e.g. Franc & Michel [29], Brennen [11], and Arndt [1]). In order take into account these effects, more sophisticated models need to be utilized, which, however, are not considered in this thesis.

There are different types of cavitation, which include traveling bubble cavitation, attached or sheet cavitation, cloud cavitation, shear cavitation, and vortex cavitation. The main focus of the thesis is on the numerical simulations of vortex cavitation. The numerical method is also applied to predict the dynamics of sheet cavitation. In section 1.1.1 vortex cavitation is described, and the other types of cavitation are described in the following [11, 29]:

- Traveling bubble cavitation (see Figure 1.3). This type of cavitation occurs when bubbles appear in the low pressure zones of the flow field as a result of the rapid growth of small air nuclei, which are the weak spots of the liquid. The bubbles are carried along by the flow, and downstream of the low pressure zone they disappear, where convecting into regions with a higher pressure.
- Attached or sheet cavitation. When a low pressure region is formed close to the leading edge of a hydrofoil, i.e. a streamlined hydrofoil in the flow, sheet cavitation

Figure 1.3: Traveling bubble cavitation on the surface of a NACA 4412 hydrofoil at zero AOA, a free-stream velocity of 13.7 m s^{-1} , and a cavitation number of 0.3 [11].

Figure 1.4: Schematic of the vapor shed cycle in sheet cavitation [68].

Figure 1.5: Combined sheet and cloud cavitation in flow about a NACA 16012 hydrofoil at 6 deg AOA, at a Reynolds number of $Re = 6 \times 10^5$, and a cavitation number of $\sigma = 0.81$ [30].

may form. The cavity is attached to the wall in a quasi-permanent way. However, this should not be accounted for as a steady behavior, because sheet cavitation is a completely unsteady phenomenon. There are several literature studies on sheet cavitation, some of them include: Franc & Michel [31, 32], Dang & Kuiper [23], Labertaux & Ceccio [72], Foeth & van Terwisga [27], and Koop & Hoeijmakers [67].

In Figure 1.4 schemataic of a sheet cavitation cycle is presented. In Figure 1.4 (a) the sheet cavity is developing, and a vapor cloud that has been formed in the previous shedding cycle is traveling in downstream direction. In Figure 1.4 (b) the sheet cavity is formed, and the vapor cloud from the previous cycle has disappeared when it entered the regions with higher pressures. The pressure inside the developed vapor sheet equals $p_{sat}(T)$, which is the lowest value of the pressure on the foil. The liquid flow around the (relatively low-pressure) vapor cavity forms a reentrant jet that travels upstream along the hydrofoil surface (towards the low pressure region) carrying a small quantity of liquid inside the cavity (see Figure 1.4 (c)). Then, as shown in Figure 1.4 (d), the reentrant jet impinges on the surface of the cavity, and part of the sheet cavity tends to detach from the surface. In Figure 1.4 (e) the vapor has shed from the main structure forming a pocket (or cloud) of vapor, which is convected with the flow. Finally, Figure 1.4 (f) shows that the vapor cloud travels downstream where it eventually disappears in the region in which the pressure is higher. Furthermore, the figure shows that a new sheet cavity is forming and a new vapor shedding cycle has started.

Figure 1.5 shows an example of sheet and cloud cavitation around a NACA 16012 hydrofoil at 6 deg AOA, at a Reynolds number of 6×10^5 , and a cavitation number

Figure 1.6: An example of shear cavitation in the wake of a wedge (as a bluff body) [28].

of 0.81 [30]. The length and thickness of the vapor sheet may vary as a function of the cavitation number and the angle of attack of the hydrofoil (see [32]). However, for this relatively thin hydrofoil the influence of the Reynolds number on cavitation is not significant [30].

- Cloud cavitation (see Figure 1.5). The periodic process of appearance and disappearance of a cloud of vapor bubbles is termed cloud cavitation. For example, when a vapor sheet detaches from the surface of a hydrofoil and is advected with the flow, the cloud of vapor structures forms downstream of the flow. When disappearing near a surface, cloud cavitation usually results in erosive effects.
- Shear cavitation (see Figure 1.6). This type of cavitation is observed in the wake of bluff bodies, in submerged liquid jets, and in separated flow regions, which develop on hydrofoils at large angles of attack. Shear cavitation forms in regions in which high levels of shear vorticity is produced. As a result more or less coherent vortical structures are formed. The pressure level drops in the core of the developed vortices, where cavitating structures may appear.

1.1.1 Vortex cavitation

Vortex cavitation usually occurs in flows at high Reynolds number containing a region of concentrated vorticity, i.e. a vortex core or filament. Inside the vortex core the pressure is often significantly lower than in the rest of the flow [11].

Vortex cavitation can be categorized into two types: well-shaped cavitating vortices, and cavitating vortices in (turbulent) shear flows [29]. The well-shaped cavitating vortices are common in fluid machinery and hydraulic structures, in tip vortices of pump impellers and ship propellers, and in the clearance passages of pumps and turbines, hub vortices trailing downstream of a propeller hub, etc [1, 11, 29]. Examples of vortex cavitation in shear flows include the alternate Bénard-von Kármán vortices behind bluff bodies, the vortices formed in shear layers at the edges of wakes and jets and the vapor filaments shed by developed cavities [29].

In this thesis, we consider the case of well-shaped cavitating vortices. In particular, we investigate the dynamics of tip vortex cavitation in the flow around a hydrofoil. The tip vortex cavitation can be viewed as a canonical problem that captures many of the essential physics associated with different types of vortex cavitation (Arndt *et al.* [2]). In

Figure 1.7: Examples of tip vortex cavitation: (a) flow about an elliptic hydrofoil [11]; (b) behind a propeller [137].

Figure 1.8: Schematic of tip vortex formation for a three-dimensional flow about an elliptic planform [29].

Figure 1.7 examples of tip vortex cavitation for an elliptic hydrofoil and behind a propeller are presented.

In the following, the formation of the tip vortex cavitation is described from a general point of view, i.e. for a flow with or without cavitation (based on [29]). Figure 1.8 shows a schematic of the non-cavitating three-dimensional flow about an elliptic planform. For a positive angle of attack, the pressure on the lower (pressure) side is higher than that on the upper (suction) side and a spanwise distribution of circulation is generated around the foil. At the tip, this pressure difference must vanish and thus the span-wise circulation also vanishes. Hence, the variation of the span-wise circulation ranges from a maximum value at the midspan section to zero at the tip of the planform.

For a large enough aspect ratio, AR , of the foil, with $AR = \frac{(\text{span length})^2}{\text{planform area}}$, the lifting line theory of Prandtl can be used to model the flow [29]. Using Prandtl's theory, the 3D flow can be modelled by a set of U-shaped line vortices (see Figure 1.8). The parts of these vortices that are attached to the foil account for the spanwise variation of circulation, whereas the free parts form a vortex sheet in the wake of the wing (Figure 1.8). This vortex sheet shown tends to roll-up because of its self-induced velocity. This mechanism leads to the formation of tip vortices.

The problem of tip vortex cavitation was first studied in detail by McCormick [87]. McCormick studied the roll-up of the trailing vortex sheet, and he established the basis of

the scaling of tip vortex cavitation inception. He related the inception to the angle of attack and the Reynolds number. Since then, extensive studies have been performed on the dynamics of the tip vortex cavitation and inception process. Some of these studies include: Billet & Holl [8], Arndt [1], Kuiper [70], Hsu [50], Maines & Arndt [84], Hart [43], Fruman [34], Keller & Rott [61], Lee & Kinnas [74], Couty, Farhat & Avellan [21], Choi, Oweis & Ceccio [16], Bulten & Opera [13], Bensow & Bark [6], Sipilä & Siikonen [123], Schot *et al.* [115], and Khatami, van der Weide & Hoeijmakers [64, 66].

1.2 Physical modeling and numerical method

1.2.1 Motivation

A computational method for compressible flow is presented in this thesis in order to perform numerical simulations of unsteady inviscid and viscous cavitating flows. Following the works of Saurel *et al.* [110], Schnerr *et al.* [114], Schmidt *et al.* [113], and Koop & Hoeijmakers [67] an equilibrium cavitation model, which is a single-fluid interface-capturing approach (see chapter 2), is adopted. This model uses Tait's equation for the liquid phase, a perfect gas equation for the vapor phase, and an equilibrium model for the mixture phase.

Computationally intensive thermodynamic relations

The governing thermodynamic relations of the employed equilibrium cavitation model are nonlinear and computationally intensive. For example, a profiling of the code used by Koop & Hoeijmakers [67] showed that nearly 90% of the computational time was spent by the routines for the computation of these thermodynamic relations. In this thesis, we replace the computationally costly thermodynamic relations by precomputed multiphase thermodynamic tables. The main objective in the construction of the tables is to prepare accurate and efficient tables (with small size of underlying data) that cover all the possible states uniquely (no need to know the phase of the flow during computations), such that the variables are looked up rapidly using a uniform spacing. However, preparing multiphase thermodynamic tables with such properties is not straightforward. The main reason is that due to a nonsmooth distribution of the data in the phase-transitioning zones of the multiphase tables, the conventional look-up procedures are inaccurate (using either linear or spline interpolation methods). The accuracy of these methods is hardly improved when using a finer grid of data points in the tables.

Discretization schemes

We perform the numerical simulations using the Unsteady Reynolds-Averaged Navier-Stokes (URANS) equations for compressible turbulent flow and using the compressible Euler equations for inviscid flow. Furthermore, we employ the Menter Shear Stress Transport (SST) model as the closure turbulence model for the URANS equations. The URANS equations alone are not sufficient to characterize the thermodynamic state of the system. To close the system of the equations, the thermodynamic state relations based on the employed equilibrium cavitation model are utilized. The method is applied to

perform numerical simulations for several test cases of non-cavitating and cavitating flow. In particular, the method is applied to perform numerical simulations of compressible flows featuring sheet and tip vortex cavitation.

We carry out the numerical simulations using a finite volume method for structured and/or unstructured grids. For the space discretization we use different schemes. One of the space discretization schemes that we employ, which is commonly used in literature, is the MUSCL family of schemes. This scheme is used for test cases of both sheet and tip vortex cavitation in this thesis. It is shown that the MUSCL schemes work well for sheet cavitation problems. However, this is not the case for tip vortex cavitation. We show that because of the high amount of numerical dissipation in the MUSCL schemes, these schemes are not well-suited for numerical simulations of vortex cavitation. To remedy this problem, extremely fine resolution of the computational grid is required for these schemes. Moreover, we show that to resolve the physics of the problem, and in order to satisfy the numerical stability, the allowed time steps are extremely small (order of nano seconds). Therefore, the need for extremely fine grids in combination with small time steps render the usage of the MUSCL schemes for efficient and accurate simulations of vortex cavitation problems impractical.

To improve the accuracy and efficiency of the spatial discretizations, we consider the higher-order accurate Weighted Essentially Non-Oscillatory (WENO) schemes. Numerical simulations employing finite volume WENO scheme of multicomponent (also cavitating) compressible flows were carried out by Johnsen & Colonius [60] for inviscid flows, and later on by Movahed & Johnsen [93], and Coralic & Colonius [20] for viscous flows. The thermodynamic model used in [20, 60, 93] is a multicomponent model (see chapter 4).

The aim of this thesis is to develop finite volume WENO schemes for cavitating flows using the employed equilibrium cavitation model (which is a single-fluid model). Although WENO schemes have proven their robustness in many applications, it is observed that for cavitating flows (with the equilibrium cavitation model) methods using the WENO scheme fail near sharp gradients and discontinuities in the flow field variables, which occur between different flow phases or near shock waves. This is due to the presence of rather small numerical oscillations near non-smooth solutions in WENO reconstruction schemes. These (small) oscillations result in non-physical values in the flow field variables such as density and/or internal energy. To avoid this issue, the numerical scheme must obey a maximum principle. Zhang & Shu [142] developed a maximum principle-preserving scheme for the higher-order accurate WENO scheme using a scaling limiter. In [142] it is shown that, in spite of using a limiter function, the higher-order accuracy of the scheme is preserved. Furthermore, it is shown in [142] that subject to a suitable (scaled) CFL condition, the scheme is numerically stable.

1.2.2 Accomplishments, and contributions

The main contributions of this thesis include:

- Development of Phase-Oriented Interpolations in Transition Cells (POITC) as a novel look-up procedure for data interpolations in the phase-transition regions of the multiphase thermodynamic tables. The POITC approach has the following features:
 - relatively simple to implement,

- fast (does not use any computationally intensive algorithm),
 - accurate,
 - allows for preparing efficient multiphase thermodynamic tables.
- Development of a novel positivity-preserving (a special case of maximum principle) strategy using logarithmic and exponential transformations for the higher-order accurate finite volume WENO scheme, denoted by log-WENO, in 1D space. The log-WENO scheme has the following features:
- rather simple,
 - does not require any limiter functions,
 - preserves the positivity property for all the points in the computational domain.

The performance of the scheme is also assessed.

- Numerical simulations of compressible inviscid and viscous flows for complex cavitation problems in 1D, 2D, and 3D using the precomputed multiphase thermodynamic tables and the POITC approach, and using different spatial discretization schemes, which are summarized in the following:
- Numerical simulations of cavitating expanding waves in 1D space using the MUSCL scheme and using higher-order accurate schemes, which include the scaling limiter maximum principle preserving WENO scheme [142], and the developed positivity-preserving log-WENO scheme.
 - Numerical simulations employing higher-order accurate multidimensional reconstruction WENO scheme for cavitating flow problems in 2D/3D space, in which the discontinuities are not strong (no need to obey the maximum principle), in particular for cavitating flow around a 2D NACA0015 hydrofoil.
 - Numerical simulations utilizing the MUSCL scheme for the flow with sheet cavitation around the 2D NACA0015 hydrofoil as well as the case of tip vortex cavitation in the flow about Arndt's elliptic hydrofoil (in 3D space).

1.3 Overview

An overview of this thesis is presented in the following. Chapter 2 provides the physical modeling of the problem. First, a review of different approaches for physical modeling of cavitation are presented, and the employed equilibrium cavitation model is described in detail. Then, the governing equations of the problem, i.e. the compressible Navier-Stokes and Euler equations, and the closure thermodynamic relations are provided. Chapter 3 describes the construction of the multiphase thermodynamic tables, and the POITC look-up procedure. Chapter 4 presents the numerical framework. First the URANS equations and the closure turbulence models are given, followed by the time and space discretization techniques. Then the verification of the methods is performed using various test problems. Subsequently, numerical simulations are reported on for compressible cavitating flow for several 1D, 2D, and 3D test cases. Finally, concluding remarks and recommendations for further extensions of the present work are provided in chapter 6.

PHYSICAL MODELING

Cavitating flows concern fluids with different phases, which possess separate mechanical and thermodynamic characteristics. The physical modeling of cavitating flows is therefore not straightforward. This is due to the physical complexities of the cavitating flows and the difficulties arising in their numerical simulations. In recent years, different cavitation models have been developed (for a comprehensive study of these models, see Koop [68]). The most common cavitation modeling approaches can be categorized into interface-tracking and interface-capturing methods. Following the works of Saurel *et al.* [110], Schnerr *et al.* [114], Schmidt *et al.* [113], and Koop & Hoeijmakers [67] the equilibrium cavitation model (which is an interface-capturing approach) is adopted in this study.

In this chapter the physical modeling of cavitating flow is presented. In the first three sections a classification of the different cavitation models is presented, and the relevant assumptions are discussed in order to motivate the use of the equilibrium cavitation model. Then the equations that are used for the numerical simulation of cavitation in this thesis are described. The Navier-Stokes and Euler equations of motion for compressible flow are presented. The governing equations of motion are not sufficient for characterizing the thermodynamic state of the system. Additional thermodynamic equations are required to close the system of equations. These closure relations for the liquid, vapor, mixture, and saturation states are presented in the subsequent parts of this chapter. Furthermore, the thermodynamic inconsistencies of the exploited model, especially with respect to the speed of sound, and their influence on the numerical simulations are discussed.

2.1 Interface-capturing vs. interface-tracking

Besides using the mass, momentum, and energy conservation laws for the numerical simulation of cavitating flow, the interface-tracking methods employ an additional numerical step in order to identify and reconstruct the interface between different phases. Some of the most common interface-tracking approaches are the diffuse-interface method (first introduced by Van der Waals [129] and later extended by Hohenberg & Halperin [49]), the phase-field method (Cahn & Hilliard [14]), the Volume-of-Fluid (VOF) method (Hirt & Nichols [47]), the level-set method (Osher & Sethian [94]), and the Discrete bubble method (Plesset & Prosperetti [98]). Furthermore, the interface-tracking methods are either Lagrangian, which employ moving grids (e.g. see Scardovelli & Zaleski [111]) or Eulerian, which use fixed meshes (e.g. the VOF and the level-set methods). The interface-tracking methods are rather accurate for small size problems such as the case of

a single bubble moving in a liquid. However, for more complex problems (e.g. a cluster of bubbles) they can be extremely computational-intensive and therefore impractical to be used.

In contrast to the interface-tracking methods, the interface-capturing methods do not need any additional numerical steps for detecting the location of the phase-interfaces. Furthermore, these methods can capture the dynamic creation of the interfaces. The interface-capturing approaches are computationally less demanding than the interface-tracking methods. Therefore they are better suited for dealing with complex multiphase problems. The interface-capturing methods are categorized into two major groups, i.e. , homogeneous-mixture (single-fluid) models and multicomponent models. Both are discussed in the following sections.

2.2 Homogeneous-mixture models

The homogeneous-mixture models treat the fluid inside the entire computational domain as a compressible flow of a single medium. In contrast to the two-fluid or multicomponent methods, which describe each phase by using separate sets of equations of motion, the homogeneous-mixture models use only one set of equations for the whole domain (a less expensive approach). These models assume that there is no slip velocity between the different phases, and that the different phases share unique density, pressure, and temperature fields. However, the accurate modeling of these unique field variables in the cavitating flow regions is not so straightforward. Some of these models (such as e.g. the barotropic flow model) employ simplified relations in order to obtain a relatively smooth distribution of the flow field variables. However, when using the more complicated models (such as the equilibrium cavitation model), which provide a more consistent and accurate formulation, often numerical difficulties are encountered. The main problem is due to sharp gradients and discontinuities in the flow field variables such as density, pressure, and speed of sound. The numerical simulations of such complex flows is thus not so straightforward, especially when higher-order accurate numerical simulations are required. In the following, some of the most common homogeneous-mixture flow models are described.

2.2.1 Transport equation-based methods (TEM)

The Transport Equation-based Methods (TEM) are considered as non-equilibrium methods. In these methods the effects of non-equilibrium phase change are taken into account. In combination with the equations for conservation of mass, momentum, and energy they employ an additional transport equation for treating the mass transfer between the phases. The transport equation in these methods can be used for the volume or mass fraction of liquid or vapor. Furthermore, the pressure, velocity, and temperature of the different phases are assumed equal, i.e., the homogeneous mixture assumption. Moreover, the phase transitions are modeled by including the rate of phase transfer as source terms in the transport equation. The advantage of the transport equation-based methods is that the unsteady flow effects of the mass transfer can be taken into account through the empirical relations for the rate of phase transition in the source term. However, the choice of the constants in the empirical relations appears to be somewhat arbitrary. Two

major classes of transport equation-based methods include: the two-phase bubble models and mass transfer rate models; these models are briefly discussed in the following.

- Kubota *et al.* [69] used a formulation that relates the density of the mixture to the motion and the dynamics of vapor bubbles in the flow. Cavitation is thus modeled as a process of the growth and collapse of vapor bubbles. The bubbles originate from the nuclei, which are introduced in the bulk flow as an initial condition. The bubbles then grow or collapse depending on the surrounding flow conditions, e.g. pressure and temperature. The evolution of the vapor bubbles is governed by the Rayleigh or Rayleigh-Plesset equation ([101], [97]).
- Merkle *et al.* [91] developed a pressure-based approach, which takes into account the mass transfer between the phases by using source terms representing vaporization/condensation. Their source terms have proven to be rather flexible for cavitation modeling. Furthermore, they offer the possibility to include the unsteady flow effects in the mass transfer between the phases. One of the drawbacks of this approach is that there are significant differences in the value of the empirical constants chosen by different authors.

Besides the approaches based on the bubble dynamics or the empirical mass transfer rates, there are also some transport equation-based methods, which take into account thermodynamic considerations for the source terms. See for example Iben *et al.* [52] and Berg *et al.* [7]. In these methods, the full set of equations for conservation of mass, momentum and energy for the mixture are solved in combination with the continuity equation for the vapor or the liquid. To close the system of equations appropriate equations of state for the liquid/vapor phase and the mixture phase must be added, which results in a system of equations accounting for two different pressures. Furthermore, care should be taken that the hyperbolicity of the resulting system of equations is preserved.

2.2.2 Bartropic flow models

Delannoy & Kueny [24] employed a barotropic relation $\rho(p)$ for the density as a function of the pressure in order to model cavitation. The function $\rho(p)$ varies within the ranges of the liquid density through a relatively smooth transitional zone to the ranges of the vapor density. The barotropic model has some advantages over the more complicated models such as e.g. an equilibrium cavitation model, which are discussed in the following. Due to a relatively smooth distribution of the field variables, the numerical solution is less difficult to obtain. Furthermore, due to the relatively simple thermodynamic relations it is computationally less intensive. One of the drawbacks of the barotropic model is that it is not well-suited for modeling cavitating flows with production of vorticity. The vorticity production is important in various cavitation problems (see Gopalan & Katz [36]), e.g. in cases with sheet cavitation or vortex cavitation. The vorticity production is a consequence of the generation of vorticity in continuity transport equation by the baroclinic term, $\nabla \frac{1}{\rho} \times \nabla p$ [116]. When the barotropic model is employed, the gradient vectors of the pressure and density are always parallel, therefore the baroclinic torque is always zero. Nevertheless, many researchers have applied this model utilizing different barotropic laws, see e.g. Reboud & Delannoy [102], Hoeijmakers *et al.* [48], and Arndt *et al.* [3].

2.2.3 Homogeneous equilibrium models

In homogeneous equilibrium models the assumption is made of a single-medium compressible flow. In the mixture regions of the domain these models assume a thermodynamic and mechanical equilibrium. The full set of the mass, momentum, and energy conservation laws are used to describe the flow. However, using the equations of motion is not sufficient for characterizing the thermodynamic state of the system. To close the system of equations, additional equations are needed. These closure relations are provided by the employed thermodynamic model.

Equilibrium cavitation model

The equilibrium cavitation model has been developed through the works of Saurel *et al.* [110], Schnerr *et al.* [114], and Schmidt *et al.* [113]. Here, we discuss the assumptions of the model. The governing thermodynamic relations are presented in section 2.4.2.

The equilibrium cavitation model assumes that the two-phase flow is in mechanical and thermodynamic equilibrium; that is, there is no relative velocity between the liquid and vapor parts, and the local pressure and temperature of the phases in the two-phase mixture are identical. Furthermore, the effects of dissolved gases and other impurities are neglected (pure water and pure vapor). Moreover, the cavitation threshold is at $p = p_{sat}$, i.e., the saturated vapor pressure state. It is noticed that in practice this assumption is not true for pure water (which is an assumption of the model). The reason is that pure water can withstand pressures that are much lower than the saturated vapor pressure (see e.g. Briggs [12], and Brennen [11]). In addition, flows of pure water are difficult to realize in practice [10]. The pure water assumption simplifies the model in that the metastable states in phase-change [11], [29] and the non-equilibrium effects are not modeled (see Koop [68], and Sezal [117]). However, these effects are modeled implicitly by the assumption of the existence of a cavitation threshold, which implies that in the liquid the pressure cannot be smaller than p_{sat} . Also, noting that in practical cases (with non-equilibrium effects) the cavitation threshold takes place at values close to, and smaller than p_{sat} (see e.g. [11], [29]), the $p = p_{sat}$ cavitation threshold of the model is thus a reasonably good approximation of the practical cases. Furthermore, the simplifications of the model make it computationally less expensive than the models, which take into account the non-equilibrium effects. Based on these assumptions, appropriate thermodynamic relations can be introduced for each of the possible states. Furthermore, the equations of state must preserve the hyperbolic nature of the resulting system of equations so that the pressure waves appearing in the fluid can be represented. This requires that a compressible flow model is considered for each of the phases of the fluid, i.e. the vapor, the liquid, and the mixture.

In order to close the description for the two-phase mixture and for the compressible liquid water, the physical properties are obtained using different approaches in the literature. Edwards & Franklin [25] employed the Sanchez-Lacombe equation of state for real-fluid flows and used an equilibrium assumption in the mixture region. Iga *et al.* [54] adopted the Tammann equation of state for the liquid phase, without taking into account the saturation conditions. Later on Iga *et al.* [53] extended this model to include the saturation conditions by considering a source term in the continuity equation for the vapor phase to model the two-phase flow. Ventikos & Tzabiras [132] obtained the

physical properties of water in all the phases from tabulated steam tables (based on experimental data). They used a relation with $f_{steam} = f_{steam}(p, h)$, where p and h are the independent variables denoting the pressure and specific enthalpy, respectively, and f_{steam} denotes the desired thermodynamic variable that is looked-up from the steam tables. For the computational use of the experimental data-based steam tables, they use the formulas that fit the data from these tables.

Saurel & Abgrall [109] used an approximation for the caloric equation of state for water along with the appropriate equations of state for the liquid and vapor phases. Furthermore, they used temperature-dependent curve fits for the liquid and vapor saturation states. This model, i.e. equilibrium cavitation model, is employed in this thesis. The governing thermodynamic relations of the equilibrium cavitation model are presented in section 2.4.2. However, note that these relations are nonlinear and computationally rather expensive. For example, a profiling of the code used by Koop [68] showed that more than 90% of the computational time is spent by the routines for the computation of these thermodynamic relations. Therefore, this approach is replaced by using precomputed multiphase thermodynamic tables containing the same information. However, in chapter 3 it will be shown that due to a non-smooth distribution of the data in the multiphase tables, preparing these tables is not so straightforward. Furthermore, when preparing the tables based on the conventional approaches, they are inaccurate and quite inefficient (large size of data). In chapter 3 we develop a procedure for preparing fast, accurate, and efficient multiphase tables. Pursuing this approach, the prepared tables are utilized in numerical simulations of cavitating flows in this thesis.

2.3 Multicomponent models

Multicomponent methods are utilized by many authors, see for example Baer & Nunziaio [5], Saurel & Abgrall [108], and Johnsen & Colonius [59]. In contrast to homogeneous-mixture models, the multicomponent methods treat each of the fluid components as a separate medium with its corresponding material properties. They assume that there is no mass transfer between the components of the fluid. Furthermore, an appropriate equation of state is used for coupling the counterpart fluid components. In addition, they use a non-conservative advection equation for detecting the location of the interfaces. This advection equation is used in combination with the full set of conservation equations, which results in a semi-conservative formulation. Moreover, the conservation equations are solved for each component of the fluid independently, which is computationally more expensive than the equations for the single-fluid models.

2.4 Governing equations

This section describes the equations that are utilized in the numerical simulations in this thesis. In the first subsection, the Navier Stokes and Euler equations of motion for compressible flow are described. The equations of motion are closed by additional thermodynamic equations. These closure thermodynamic relations are provided by the employed equilibrium cavitation model. In the second subsection of this section the governing thermodynamic relations for the equilibrium cavitation model are discussed. Furthermore, the consistency and uniqueness of the thermodynamic relations for the entire

thermodynamic domain of interest (which includes all the possible thermodynamic states that are defined by the governing thermodynamic relations) is investigated.

2.4.1 Navier-Stokes and Euler equations for compressible flow

The Navier-Stokes equations for compressible flow in conservation form are given by

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \vec{\mathbf{F}}_j}{\partial x_j} = \frac{\partial \vec{\mathbf{F}}_j^v}{\partial x_j}, \quad (2.1)$$

where $\mathbf{U}$ denotes the vector of the conservative variables

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u_i \\ \rho E \end{bmatrix}, \quad (2.2)$$

and $\vec{\mathbf{F}}_j$ and $\vec{\mathbf{F}}_j^v$ are the inviscid and viscous flux vectors, respectively, defined as:

$$\vec{\mathbf{F}}_j = \begin{bmatrix} \rho u_j \\ \rho u_i u_j + p \delta_{ij} \\ \rho u_j H \end{bmatrix}, \quad (2.3)$$

$$\vec{\mathbf{F}}_j^v = \begin{bmatrix} 0 \\ \tau_{ij} \\ \tau_{jk} u_k - q_{\kappa,j} \end{bmatrix}, \quad (2.4)$$

with the indices $\{i, j, k = 1, \dots, 3\}$. Here, δ_{ij} is the Kronecker delta function, H denotes the total specific enthalpy

$$H = E + \frac{p}{\rho} = h + \frac{1}{2} u_i u_i. \quad (2.5)$$

Here, E and h are the total specific energy and the specific static enthalpy, respectively, defined as

$$E = e + \frac{1}{2} u_i u_i, \quad h = e + \frac{p}{\rho}, \quad (2.6)$$

where e denotes the specific internal energy. τ_{ij} denotes the component of the shear stress tensor, which based on the Newtonian fluid assumption, is defined as follows

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k}, \quad (2.7)$$

where μ is the molecular dynamic viscosity coefficient. Moreover, $q_{\kappa,j}$ is the component of the heat flux vector that is formulated based on the Fourier's law of heat conduction as

$$q_{\kappa,j} = -\kappa \frac{\partial T}{\partial x_j}, \quad (2.8)$$

where κ is the heat conduction coefficient of the fluid. In the case of inviscid flow the Euler equations are used. The Euler equations in conservation form are expressed as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \vec{\mathbf{F}}_j}{\partial x_j} = 0, \quad (2.9)$$

which can be derived by setting the viscous fluxes in equation (2.1) equal to zero.

Table 2.1: Coefficients in the relation for the saturation state (taken from [112])

i	a_i	$\hat{a}_i$	b_i	$\hat{b}_i$	c_i	$\hat{c}_i$
1	0	0	1	0	0	0
2	-7.85823	1	1.99206	1/3	-2.02957	1/3
3	1.83991	3/2	1.10123	2/3	-2.68781	2/3
4	-11.7811	3	-0.512506	5/3	-5.38107	4/3
5	22.6705	7/2	-1.75263	16/3	-17.3151	3
6	-15.9393	4	-45.4485	43/3	-44.6384	37/6
7	1.77516	15/2	-6.75615×10^5	110/3	-64.3486	71/6

2.4.2 Equilibrium cavitation model

The equilibrium cavitation model was introduced in section 2.2.3. In this subsection, the governing thermodynamic relations of the equilibrium cavitation model for the liquid, vapor, and mixture phases and the saturation states are described.

Thermodynamic relations

Saturation state

The relations for the saturation state are obtained via the following seventh-order polynomial curve fits (Schmidt [112]):

$$\ln \left(\frac{p_{sat}(T)}{p_c} \right) = \frac{T_c}{T} \sum_{i=1}^7 a_i \theta^{\hat{a}_i}, \quad (2.10)$$

$$\frac{\rho_{l,sat}(T)}{\rho_c} = \sum_{i=1}^7 b_i \theta^{\hat{b}_i}, \quad (2.11)$$

$$\ln \left(\frac{\rho_{v,sat}(T)}{\rho_c} \right) = \sum_{i=1}^7 c_i \theta^{\hat{c}_i}, \quad (2.12)$$

where $\theta = 1 - T/T_c$, and $a_i, \hat{a}_i, b_i, \hat{b}_i, c_i, \hat{c}_i$ are the constants given in Table 2.1 (taken from Schmidt [112]). These relations are valid for the range of temperature with lower and upper limits T_0 and T_c , respectively, which are the triple point and the critical point temperatures of water, respectively. The values of the constants used in equations (2.10) - (2.12) are $T_c = 647.30$ K, $p_c = 22.12 \times 10^6$ Pa, $\rho_c = 317.0$ kg m⁻³, and $T_0 = 273.16$ K. In Figure 2.1 the plots of the saturated vapor and liquid densities and the saturated pressure are presented. These plots are obtained for the temperature range of $T_r \leq T \leq T_c$.

Figure 2.1: Plots of the saturation states: (a) saturated vapor and liquid densities; (b) saturated pressure; The plots are obtained for the temperature range of $T_r \leq T \leq T_c$, with the specified triple point (R) and the critical point (C).

Furthermore, according to Koop [68] the plots fit the experimental data with a level of accuracy that was sufficient for his purposes.

Liquid phase

Following Saurel *et al.* [110], the relation for the liquid thermal equation of state is governed by a modified Tait equation. In this equation the liquid pressure is expressed in terms of density and temperature given by

$$p_l(\rho_l, T_l) = K_0 \left[\left(\frac{\rho_l}{\rho_{l,sat}(T)} \right)^N - 1 \right] + p_{sat}(T), \quad (2.13)$$

with constants $K_0 = 3.3 \times 10^8$ Pa and $N = 7.15$ for water. Here, the variables $\rho_{l,sat}(T)$ and $p_{sat}(T)$ are the saturated liquid density and pressure, respectively, which are functions of temperature (see equations (2.11) and (2.10)).

In order to derive the caloric equation of state for the liquid phase, the thermal equation of state (equation (2.13)) and the relevant thermodynamic relations of Maxwell are utilized. From the Maxwell relations based on the independent variables (v, T) , with $v = 1/\rho$ and T denoting the specific volume and the temperature, respectively, we have

$$\left(\frac{\partial e}{\partial T} \right)_v = c_v(v, T), \quad \left(\frac{\partial e}{\partial v} \right)_T = -p + T \left(\frac{\partial p}{\partial T} \right)_v, \quad (2.14)$$

where $c_v(v, T)$ is the specific heat at constant volume. By taking the cross-derivatives of e with respect to v and T of the relations in equation (2.14), and equating the results, the following expression is obtained for $c_v(v, T)$

$$\left(\frac{\partial c_v(v, T)}{\partial v} \right)_T = T \left(\frac{\partial^2 p}{\partial T^2} \right)_v. \quad (2.15)$$

After substituting the expression for p from equation (2.13) in equation (2.15) the following expression can be derived

$$\left(\frac{\partial c_v(v, T)}{\partial v} \right)_T = T \frac{NK_0}{v^N \rho_{sat}^{N+2}} \left[(N+1) (\rho'_{sat})^2 - \rho_{sat}(T) \rho''_{sat} \right] + T p''_{sat}, \quad (2.16)$$

where the prime denotes differentiation with respect to T . The expression for c_v can thus be obtained by integrating equation (2.16). Furthermore, this relation shows that c_v is a function of both v and T and not just of one of them.

In order to derive an expression for the internal energy, e , the partial derivatives in equation (2.14) must be integrated with respect to the independent variables v and T . To do this, either one of the following integrals can be used to derive the value of a quantity $f(x, y)$ based on the the partial derivatives of f with respect to the independent variables x and y and based on a reference state (x_0, y_0)

$$f(x, y) = \int_{x_0}^x \left(\frac{\partial f}{\partial x} \right)_y (\hat{x}, y_0) d\hat{x} + \int_{y_0}^y \left(\frac{\partial f}{\partial y} \right)_x (x, \hat{y}) d\hat{y} + f(x_0, y_0), \quad (2.17)$$

$$f(x, y) = \int_{x_0}^x \left(\frac{\partial f}{\partial x} \right)_y (\hat{x}, y) d\hat{x} + \int_{y_0}^y \left(\frac{\partial f}{\partial y} \right)_x (x_0, \hat{y}) d\hat{y} + f(x_0, y_0). \quad (2.18)$$

By using this formulation and after replacing $v = 1/\rho$ and choosing a reference state (ρ_0, T_0) , the partial derivatives in equation (2.14) are integrated and the expression for $e(\rho, T)$ is derived as follows

$$\begin{aligned} e(\rho, T) = & \int_{T_0}^T c_v(\rho_0, \hat{T}) d\hat{T} + e(\rho_0, T_0) + \underbrace{\frac{(Tp'_{sat} - p_{sat} + K_0)}{\rho_0} \left(\frac{\rho_0}{\rho} - 1 \right)}_I \\ & + \underbrace{\frac{K_0}{N-1} \left(\frac{\rho_{sat}(T) + NT\rho'_{sat}}{\rho_{sat}^2(T)} \right) \left(\left(\frac{\rho}{\rho_{sat}(T)} \right)^{N-1} - \left(\frac{\rho_0}{\rho_{sat}(T)} \right)^{N-1} \right)}_{II}, \end{aligned} \quad (2.19)$$

For water, this expression can be simplified. Since, there are relatively small variations in the density of water it can be assumed that $\rho \approx \rho_0 \approx \rho_{sat}(T)$. With this assumption the terms I and II in equation (2.19) become approximately equal to zero. Furthermore, for water at room temperatures it can be assumed that $c_v(\rho_0, T) \equiv C_{vl}$ is constant. With these assumptions an approximate caloric equation of state can be obtained. In this thesis, the approximate caloric equation of state given by

$$e_l(\rho_l, T_l) = e_l(T_l) = C_{vl}(T_l - T_0) + e_{l0}, \quad (2.20)$$

is adopted from Saurel *et al.* [110], which according to Koop [68] provides a good approximation of equation (2.19) for water. The speed of sound in the liquid, c_l , is obtained from equation (2.40), which can be written as follows

$$c_l^2 = \frac{N\bar{p}(T_l)}{\rho_l} + \frac{p_l}{\rho_l^2 C_{vl}} \left(p'_{sat}(T_l) - \frac{N\bar{p}(T_l)}{\rho_{l,sat}(T_l)} \rho'_{l,sat}(T_l) \right), \quad (2.21)$$

where, $\bar{p}(T) = p_l - p_{sat}(T) + K_0$. Moreover, the prime denotes differentiation with respect to T . For water, the constants in these relations are defined as $C_{vl} = 4180 \text{ J kg}^{-1} \text{ K}^{-1}$ (the specific heat at constant volume), $T_0 = 273.16 \text{ K}$ (a reference temperature), and $e(\rho_0, T_0) \equiv e_{l0} = 617.0 \text{ J kg}^{-1}$ (a reference internal energy).

Vapor phase

The equations of state for the vapor phase are based on a calorically perfect gas model. The thermal equation of state for a perfect gas is given by

$$p_v(\rho_v, T_v) = \rho_v R_v T_v, \quad (2.22)$$

which in the case of the calorically perfect gas (with constant specific heats), can be written as

$$p_v(\rho_v, T_v) = (\gamma - 1) \rho_v e_v. \quad (2.23)$$

The caloric equation of state for the vapor phase is given by

$$e_v(T_v) = C_{vv}(T_v - T_0) + L_v(T_0) + e_{l0}. \quad (2.24)$$

Furthermore, the speed of sound c_v in vapor is derived from equation (2.40), which is given by

$$c_v^2 = \gamma \frac{p_v}{\rho_v} = \gamma R_v T_v. \quad (2.25)$$

Here, the constants with their corresponding values for water vapor are defined as $R_v = 461.6 \text{ J kg}^{-1} \text{ K}^{-1}$ (the specific gas constant) with $\gamma = 1.327$ (the specific heat ratio), $L_v(T_0) = 2.3753 \times 10^6 \text{ J kg}^{-1}$ (the latent heat of vaporization), $C_{vv} = 1410.8 \text{ J kg}^{-1} \text{ K}^{-1}$ (the specific heat at constant volume), and T_0 , and e_{l0} were defined in the preceding part for the liquid phase.

Note that for equations (2.22), and (2.24) the consistency of these relations with the saturation state equations, i.e. equations (2.10), (2.11), and (2.12), is not taken into account. To assess the inconsistency of the relations, the vapor caloric and thermal equations of state, which are consistent with the saturation state, are derived in the following. Considering a reference state $\tilde{e}_{v0} \equiv \tilde{e}_v(\rho_{v0}, T_0)$, the caloric equation of the state for the vapor phase is given by

$$\tilde{e}_v(\rho_v, T_v) \equiv \tilde{e}_v(T_v) = C_{vv}(T - T_0) + \tilde{e}_{v0}, \quad (2.26)$$

where, the double tilde sign denotes the variables, which are consistent with the saturation states. In this equation, the reference state $\tilde{e}_{v0}$ is unknown, which is to be determined in

the following. For the reference state with $T = T_0$ in the liquid saturation state we have

$$T_l = T_0, \rho_l = \rho_{l,sat}(T_0), \quad (2.27)$$

$$h_{l0} = e_{l0} + \frac{p_{sat}(T_0)}{\rho_{l,sat}(T_0)}, \quad (2.28)$$

where h_{l0} is the specific enthalpy of the liquid water in the reference state. The specific enthalpy of the water vapor in the reference state, i.e., h_{v0} can be computed by adding the latent heat of vaporization to h_{l0} , therefore we have

$$T_v = T_0, \rho_v = \rho_{v,sat}(T_0), \quad (2.29)$$

$$\begin{aligned} \tilde{h}_{v0} &= \tilde{e}_{v0} + \frac{p_{sat}(T_0)}{\rho_{v,sat}(T_0)} \\ &\equiv h_{l0} + L_v(T_0) = e_{l0} + \frac{p_{sat}(T_0)}{\rho_{l,sat}(T_0)} + L_v(T_0). \end{aligned} \quad (2.30)$$

From this equation, the following expression is obtained for $\tilde{e}_{v0}$

$$\tilde{e}_{v0} = e_{l0} + L_v(T_0) + p_{sat}(T_0) \left(\frac{1}{\rho_{l,sat}(T_0)} - \frac{1}{\rho_{v,sat}(T_0)} \right). \quad (2.31)$$

Therefore, the equation (2.26) can be rewritten as follows

$$\tilde{e}_v(T_v) = C_{vv}(T_v - T_0) + L_v(T_0) + e_{l0} + p_{sat}(T_0) \underbrace{\left(\frac{1}{\rho_{l,sat}(T_0)} - \frac{1}{\rho_{v,sat}(T_0)} \right)}_{\tilde{e}_{v,extra}}. \quad (2.32)$$

By using the equations (2.32) and (2.22) we get

$$\tilde{e}_v(T_v) = C_{vv}T_v + \underbrace{(L_v(T_0) + e_{l0} + \tilde{e}_{v,extra} - C_{vv}T_0)}_{\tilde{e}_{v,rest}} \quad (2.33)$$

$$= \frac{C_{vv}}{R_v} \frac{\tilde{p}_v}{\rho_v} + \tilde{e}_{v,rest} = \frac{1}{\gamma - 1} \frac{\tilde{p}_v}{\rho_v} + \tilde{e}_{v,rest}. \quad (2.34)$$

Using this expression and by replacing $\tilde{e}_{v,rest}$ and $\tilde{e}_{v,extra}$ the following expression is derived for p_v

$$\begin{aligned} \tilde{p}_v &= (\gamma - 1) \rho_v \tilde{e}_v(T_v) \\ &\quad - (\gamma - 1) \rho_v \left(p_{sat}(T_0) \underbrace{\left(\frac{1}{\rho_{l,sat}(T_0)} - \frac{1}{\rho_{v,sat}(T_0)} \right)}_{\tilde{p}_{v,extra}} + L_v(T_0) + e_{l0} - C_{vv}T_0 \right). \end{aligned} \quad (2.35)$$

In the following, the relative differences between the values obtained from the equations that are used for the numerical simulations in this thesis, and the values from the alternative relations, which are consistent with the saturation states, are discussed. The relative error function $\tilde{E}(x, y)$ corresponding to the variables x and y is defined by

$$\tilde{E}(x, y) = \left| \frac{y - x}{y} \right|. \quad (2.36)$$

It was found that the maximum relative error $\tilde{E}_{max}$ corresponding to the values of the caloric equations of state obtained from equations (2.24) and (2.32) is orders of percents, i.e. $\tilde{E}_{max}(e_v, \tilde{e}_v) = O(10^{-2})$.

Moreover, for the thermal equations of state obtained from equations (2.22) and (2.35) it was found that $\tilde{E}_{max}(p_v, \tilde{p}_v) = O(10^{-4})$. Note that these errors are not entirely due to the inconsistency of the relations. The curve fit of the saturation state also contributes to the magnitude of these errors. Moreover, compared to the approximation errors associated with the modeling of cavitation these errors are expected to be negligible. Note that the vapor phase relations (2.22), (2.24), and (2.25) are the ones that are used in thesis.

Mixture phase

For the equilibrium cavitation model it is assumed that there is a thermodynamic equilibrium in the mixture phase. This implies that the values of the mixture pressure and mixture temperature remain equal to their values in the saturation states, that is,

$$p = p_{sat} \quad \text{and} \quad T = T_{sat}. \quad (2.37)$$

The mixture density ρ is expressed as

$$\rho = \alpha \rho_{v,sat}(T) + (1 - \alpha) \rho_{l,sat}(T), \quad (2.38)$$

and the caloric equation of state is defined by

$$\rho e = \alpha \rho_{v,sat}(T) e_v(T) + (1 - \alpha) \rho_{l,sat}(T) e_l(T), \quad (2.39)$$

where α is the vapor void fraction, i.e., $\alpha = 1$ for pure vapor and $\alpha = 0$ for pure liquid. The saturation pressure and density are functions of the temperature only (see equations (2.10), (2.11), and (2.12)). Moreover, the mixture speed of sound $c_{mix} \equiv c$ is obtained from the Wallis [133] formula (equation (2.41)).

Speed of sound

The acoustic speed of sound c can be obtained from an eigenvalue analysis of the system of equations (2.9). The expression for c , based on the independent variables (ρ, e) , is derived as follows (for derivation of the formula see Appendix A.1):

$$c^2 = \left(\frac{\partial p}{\partial \rho} \right)_e + \frac{p}{\rho^2} \left(\frac{\partial p}{\partial e} \right)_\rho. \quad (2.40)$$

In Figure 2.2, a plot of the acoustic speed of sound (equation (2.40)) for a constant temperature of $T = 298$ K covering all the possible states is presented. The plot shows that there is a discontinuity in the speed of sound when transitioning from the liquid to the mixture phase, which is not a desirable property for numerical simulations (see Sezal [117]). Also the transition from the mixture to the vapor phase is not continuous, albeit much less severe. The rather low values of the speed of sound for small values of α

Figure 2.2: Speed of sound c plots (in logarithmic scale) vs. vapor void fraction α at $T = 298$ K, for acoustic speed of sound (equation (2.40)), and the Wallis formula (equation (2.41)).

can also lead to numerical problems. Therefore, the Wallis [133] formula for the speed of sound is employed in the mixture phase:

$$\frac{1}{\rho c^2} = \frac{\alpha}{\rho_{v,sat}(T) c_v^2} + \frac{1 - \alpha}{\rho_{l,sat}(T) c_l^2}, \quad (2.41)$$

where, c_v and c_l are the speed of sound in the vapor and liquid, respectively, which are computed from equation (2.40). In Appendix B aspects of using the Wallis speed of sound in numerical simulations are discussed. Furthermore, the feasibility of using the acoustic speed of sound in the entire domain is investigated.

The equations of state introduced for the three phases in combination with the saturation state cover all possible thermodynamic equilibrium states within their corresponding ranges of definition. To show this, sample plots of the variables that are obtained using the thermal equations of state (equations (2.13), (2.22), and (2.37)) and the caloric equations of state (equations (2.20), (2.24), and (2.39)) are presented in Figure 2.3, and Figure 2.4, respectively. Figure 2.3 shows pressure p versus specific volume $v = 1/\rho$ (for a constant temperature of $T = 298$ K) covering all the possible states. Koop [68] showed that the level of agreement between Figure 2.3 and experimental data was sufficient for his purposes.

Furthermore, Figure 2.4 shows the cross-section plots of the internal energy e versus the temperature T for constant density ρ . The plots are obtained based on the ranges of the variables that are used in the numerical simulations in this thesis. In this figure, the results in the mixture phase are shown by the curved lines. Additionally, the bounding lines at the top and bottom of the figure correspond to the thermodynamic states for which the caloric equation of state is independent of the density. These states include the vapor/saturation state (top green line), and the liquid/saturation state (bottom red

Figure 2.3: State plot of pressure p vs. specific volume v (in logarithmic scale) at $T = 298$ K. The constant temperature line (solid line with symbols) is plotted for liquid, mixture, and vapor phases.

Figure 2.4: Sample plots of constant density curves for internal energy e vs. temperature T . The plots are obtained for $273.1 \leq T \leq 350$, $2 \times 10^{-6} \leq \rho \leq 1100 \text{ kg m}^{-3}$, and the corresponding values of e .

line). Furthermore, it is observed that the curves for the mixture plotted in Figure 2.4 are monotonically increasing without intersecting each other, i.e., there is a unique relation between the $\{\rho, e, T\}$ variables. This shows the uniqueness of the thermodynamic relations for these variables. We further discuss the consistency and uniqueness of the thermodynamic relations in the next section. Finally, the gradients of the employed

thermodynamic relations in all the phases using the independent variables (ρ, e) are presented in Appendix C. These gradients are required for the computation of the speed of sound, for the characteristic-wise decomposition of Navier-Stokes equations, etc.

2.4.3 Consistency and uniqueness of thermodynamic relations

For the thermodynamic relations introduced in the preceding section, we show in this section that these equations provide a nearly consistent and unique formulation that covers all the possible states. We begin by rewriting the caloric equation of state for the mixture phase (equation (2.39)) as

$$e(\rho, T) = \frac{\alpha \rho_{v,sat}(T) e_v(T) + (1 - \alpha) \rho_{l,sat}(T) e_l(T)}{\rho}. \quad (2.42)$$

Noting that for the density ρ of the mixture, the relation $\rho_{v,sat} \leq \rho \leq \rho_{l,sat}$ holds, from equation (2.42) we get $e(\rho_{l,sat}, T) \equiv e_{l,sat} = e_l(T)$, and $e(\rho_{v,sat}, T) \equiv e_{v,sat} = e_v(T)$. Furthermore, from equation (2.20) and equation (2.24), it follows that for the range of temperature $T_0 \leq T \leq T_c$, we have $e_v(T) > e_l(T)$ at a constant temperature, and that using equation (2.42) the following inequality holds:

$$e_l(T) \leq e(\rho, T) \leq e_v(T), \quad (2.43)$$

This inequality shows that the caloric equations of state in the current study cover all the possible thermodynamic states consistently and with unique values.

To check whether these properties also hold for the speed of sound c , we rewrite equation (2.41) as a function of a mapped variable $\xi = \frac{1}{c^2}$, which yields

$$\frac{1}{\rho} \xi(c) = \frac{\alpha}{\rho_{v,sat}(T)} \xi_v(c_v) + \frac{1 - \alpha}{\rho_{l,sat}(T)} \xi_l(c_l). \quad (2.44)$$

From this equation, it is evident that $\xi(c_{v,sat}) = \xi_v(c_{v,sat})$ and $\xi(c_{l,sat}) = \xi_l(c_{l,sat})$; that is, the values of the ξ in the mixture phase are bounded by the values of ξ_v and ξ_l . Therefore, the relations for the speed of sound are also consistent and unique. In section 3.3 it is shown that in order to obtain an accurate look-up procedure for c , it is important to perform the interpolations for $\xi(c)$ rather than for c itself.

Concerning the thermal equations of state, it follows that the relations for the liquid and the mixture phases, that is, equation (2.13) and equation (2.37), respectively, are consistent and possess unique values. However, due to the curve fit error in the saturation states (equation (2.10)), there is a minor inconsistency between the thermal equations of state for the vapor phase and the mixture phase, that is, when equations (2.22) and (2.37) are evaluated at the transition from mixture to vapor, slightly different values are obtained. Figure 2.5 shows the relative inconsistency for the pressure in the saturation state between the mixture and vapor. The relative error is denoted by $\tilde{E}(p_v^{v,sat}, p_v^{v,sat})$, where $p_v^{v,sat}$ and $p_v^{v,sat}$ are the values of pressure in the saturation vapor state obtained from the relations in the mixture phase and those for the vapor phase. The values of the saturation vapor density $2 \times 10^{-6} \leq \rho_{v,sat}(T) \leq 0.3 \text{ kg m}^{-3}$ in Figure 2.5 are derived for temperatures of $273.1 \leq T \leq 350 \text{ K}$ (the temperature range in our simulations), which cover the entire saturation vapor state in this range. Therefore, disregarding this minor inconsistency (caused by a fitting error, i.e., no fundamental issue), it can be concluded that the thermodynamic state of the system is defined consistently and uniquely by the utilized equations of state.

Figure 2.5: Relative error of inconsistency $\tilde{E}_{p_{v,sat}}$ of the saturated vapor pressure in the formulations for the mixture phase and the vapor phase (logarithmic scales). Here, $2 \times 10^{-6} \leq \rho_{v,sat}(T) \leq 0.3 \text{ kg m}^{-3}$ for $273.1 \leq T \leq 350 \text{ K}$.

MULTIPHASE THERMODYNAMIC TABLES

The thermodynamic relations discussed in section 2.4.2 are nonlinear and computationally intensive. For example, a profiling of the code used by Koop & Hoeijmakers [67] showed that nearly 90% of the computational time was spent by the routines for computation of the thermodynamic relations. In this thesis, the computationally costly thermodynamic approach is replaced by using precomputed multiphase thermodynamic tables. It is aimed to prepare accurate and efficient tables (with limited amount of data) that cover all the possible states uniquely (no need to know the phase of the flow during computations), such that the variables are looked up rapidly (accomplished by uniform spacing). However, preparing multiphase tables with such properties is not straightforward. The main reason is that due to a nonsmooth distribution of the data in the phase-transitioning zones of the multiphase tables, the conventional look-up procedures using either linear or spline interpolation methods are inaccurate. The accuracy of these methods is hardly improved when using a finer grid of the data points for preparing the tables.

There are few studies in the literature that have investigated the computational use of the thermodynamic tables with different phases. Azimian *et al.* [4] employed artificial neural networks (ANN) for generating steam tables. Miyagawa & Hill [92] developed the Tabular Taylor Series Expansion (TTSE) method for the calculation of water and steam properties. Kunick *et al.* [71] introduced a table look-up method based on two-dimensional spline functions. In all of these papers either the phases are considered separately or, if the phases are considered simultaneously, the treatment of the discontinuous data in the phase-transitioning regions is not well addressed. Wang *et al.* [134] and Gräber *et al.* [38] developed spline-based look-up methods with an emphasis on the discontinuous data in the phase-transitioning regions. They managed to improve the accuracy of the tables compared to the previous studies in [92], and [71].

In this chapter, the procedure for preparing the multiphase thermodynamic tables is described. Different aspects of the preparation of the tables are discussed, such as the procedure for the data interpolations from the constructed tables. Then, the failure of the conventional interpolation methods in providing accurate results for multiphase tables is discussed. Finally, the Phase-Oriented Interpolations in Transition Cells (POITC) is developed as a novel interpolation approach. It is shown that when using POITC, much more efficient (much smaller size) multiphase tables can be prepared compared to the conventional approaches. Furthermore, it is shown that by using POITC the look-up procedure is fast (almost instantaneous) and the accuracy of the interpolations is significantly improved compared to the accuracy of the conventional interpolation approaches. In this thesis, the nondimensional variables $\zeta = \frac{e}{e_\zeta}$ and $\eta = \frac{\rho}{\rho_\eta}$ are used for

the internal energy e and the density ρ , respectively. The reference variables are taken as $\rho_\eta = 1100 \text{ kg m}^{-3}$ and $e_\zeta = 2.48433698 \times 10^6 \text{ J kg}^{-1}$, which are the maximum values of ρ and e in the constructed thermodynamic tables.

3.1 Preparing the tables

In the following the procedure for preparing the multiphase thermodynamic tables, and the data interpolations in these tables is described ¹. In section 2.4.3 it is shown that the employed thermodynamic relations cover all the possible states consistently and uniquely. Due to the consistency and uniqueness of the thermodynamic relations, they can be used to prepare unique multiphase tables for the desired thermodynamic variables for all possible thermodynamic states. It is intended to prepare two-dimensional thermodynamic tables using a pair of independent variables on a structured grid of data points containing the desired thermodynamic variables. In this thesis, the pair of independent variables (ρ, e) , i.e. density and internal energy, are used for preparing the tables. The main reason is that this pair of variables can be obtained directly from the conservative variables in the numerical simulations, which is computationally efficient. However, at some stages of the numerical simulations, only the pair of primitive variables (from which ρ or e cannot be computed directly) such as e.g. (ρ, p) or (T, p) with p and T denoting the pressure and the temperature, respectively, are known. In such cases, the desired independent variable ρ or e is computed using an iterative algorithm (e.g. Newton's algorithm).

Two-dimensional (ρ, e) -based multiphase thermodynamic tables are prepared, which contain data for the primitive variables $\Psi = \{p, T, c, \alpha\}$, that is, pressure, temperature, speed of sound and vapor void fraction. The constructed tables are composed of uniform cells, with each cell consisting of four data nodes. Interpolation of the desired thermodynamic variable is performed within the cell. A schematic representation of a multiphase table is shown in Figure 3.1a. The table covers all the possible states, that is, vapor, mixture, and liquid phases, and also the phase transition between mixture-vapor and mixture-liquid. From a general perspective, the multiphase tables are composed of cells that contain either uniform-phase data (vapor or mixture or liquid phases) or nonuniform-phase data (phase-transitioning zones). A schematic of a phase-transition cell is shown in Figure 3.1b. The two different phases (here, mixture and liquid) are separated by the liquid saturation curve (the dotted line).

In a cavitating flow, the density range is varying from rather low values (vapor) to high values (liquid). Moreover, the internal energy can also attain a variety of ranges when comparing the parts with low densities to the ones with high densities. Due to the widespread ranges of density and internal energy, preparing a single $\rho - e$ table with uniform ρ and e step sizes will be either inaccurate or very inefficient (impractically large size). Furthermore, one may consider using logarithmic scales for grid spacings to solve this problem. Although when using the logarithmic scales a smoother grid of data points can be used. However, in the present study it has been found that utilizing a logarithmic grid spacing does not result in the desired level of accuracy. Moreover, the logarithmic transformations increase the computational costs. Therefore, the logarithmic grid spacing was not considered further in this thesis.

¹Part of the contents of this section is based on Refs. [65], [63], and [62]

Figure 3.1: Schematic of: (a) $\rho - e$ multiphase table (the highlighted cells are the phase-transitioning cells); (b) a phase-transitioning cell with the data nodes in the mixture region (O), the liquid region (x), the sample state point (●), and with the saturation curve (dotted line).

3.1.1 Splitting the tables

For the sake of efficiency, the table for each thermodynamic variable was split in different subtables, each with a different equidistant spacing. The split is in terms of ρ , with temperature ranges of $T_{min} \leq T \leq T_{max}$ and the corresponding ranges of e . This results in different ρ and e step sizes for each region. In order to keep consistency at the boundaries between the subtables, the subtables overlap. In Figure 3.2a, sample plots of the regions of the three neighboring subtables m, n, l are presented (each region highlighted in different color). The subtable boundaries are constant ρ curves, in $T - e$ space. Furthermore, the overlap regions between the subtables are visible in the same figure. Note that the highlighted regions in Figure 3.2a, do not represent the entire domain of the subtables. In each subtable, there are some regions that are undefined. The reason for this is explained in the following.

In order to prepare each subtable a two dimensional uniform grid of the data is used with the independent variables ρ and e on the vertical and horizontal axes, respectively. The grid spacing on the axis of each subtable is computed based on the ranges of ρ and e in that subtable, with $\rho_{min} \leq \rho \leq \rho_{max}$ and $e_{min} \leq e \leq e_{max}$ and using the desired

Figure 3.2: Sample plots of the subtable regions: (a) neighboring subtable regions in $T - e$ space for subtables m, n, l . Each subtable is bounded by two constant ρ curves, and overlaps with its neighboring subtable (the striped areas); (b) a subtable m , with ρ boundaries $\rho_{\min}$ and $\rho_{\max}$, the e and T boundaries specified by the dotted lines, and with the undefined regions that are highlighted; The green and red lines on the top and the bottom of the plots show the vapor and liquid phases, respectively.

number of data points n_ρ and n_e , such that

$$\Delta\rho = \frac{\rho_{\max} - \rho_{\min}}{n_\rho}, \quad \Delta e = \frac{e_{\max} - e_{\min}}{n_e}. \quad (3.1)$$

Here, $\Delta\rho$ and Δe are the grid spacings on the ρ and e axis, respectively. Moreover, in each subtable the ranges of temperature are $T_{\min} \leq T \leq T_{\max}$. For each subtable, the ranges of ρ and T are predefined. However, the range of e is not known apriori. Thus, using the known values ρ and T , the ranges of e , i.e., $(e_{\min}, e_{\max})$ are determined. Then, based on the known (ρ, e) ranges in each subtable, the tables are prepared. However, part of the regions in some of the subtables correspond to the thermodynamic states with temperatures that are not within the defined bounds of T and are therefore flagged as undefined. Figure 3.2b shows the entire region of a sample subtable plotted in $T - e$ space, which includes both the defined and undefined parts. The undefined regions of the subtable are highlighted in this figure, and the boundaries of the actual ranges of e and T are shown by dotted lines. When storing the data for the subtables, the areas that are not defined for that subtable are flagged as undefined and therefore are not taken into account in the computations.

We will discuss the interpolation of the data in the subtables in sections 3.2 and 3.3. However, regardless of the interpolation approach that is used in the subtables, in order to preserve the consistency of the interpolated data in the overlapping regions an additional step is carried out for these regions. This step is carrying out a weighted averaging of the interpolated data from the overlap regions of the neighboring subtables. Figure 3.3 shows a schematic of the ranges of the density ρ for two neighboring subtables that overlap. The indices m and n represent the neighboring subtables with an overlapping region denoted

Figure 3.3: Schematics of the overlapping zone: (a) the density ranges of two neighboring subtables; data points used for computation of (b) $\left(\frac{\partial\Psi}{\partial\rho}\right)_e\Big|_1$, (c) $\left(\frac{\partial\Psi}{\partial e}\right)_\rho\Big|_1$.

by the index mn . It is assumed that $\rho_m^a \leq \rho_m \leq \rho_m^b$ and $\rho_n^a \leq \rho_n \leq \rho_n^b$ for the subtables m , and n , respectively, for which the superscripts a and b are the starting and ending values of the domain, respectively. The thermodynamic data in the overlapping region, denoted by Ψ_{mn} , are obtained as follows:

$$\Psi_{mn} = \beta\Psi_m + (1 - \beta)\Psi_n, \quad (3.2)$$

where β is the averaging weight, such that

$$\beta = \frac{\rho_{mn} - \rho_m^b}{\rho_n^a - \rho_m^b}. \quad (3.3)$$

3.1.2 Gradients' look-up

In Appendix C, the analytical expressions for the gradients of the employed thermodynamic relations in each of the phases are presented. However, due to the consistency and uniqueness of the prepared thermodynamic tables, the gradients of the thermodynamic variables can also be interpolated from these tables. In this thesis, the partial derivatives of a variable Ψ with respect to the independent variables $\psi = \{\rho, e\}$ are interpolated using two methods, namely, finite element-like approximations, and a perturbation method. In the finite element approach, the partial derivatives $\left(\frac{\partial\Psi}{\partial\rho}\right)_{e,m}$ and $\left(\frac{\partial\Psi}{\partial e}\right)_{\rho,m}$ at a state point (ρ, e) inside a cell of subtable m are computed using bilinear element approximations in that cell.

In the perturbation method, the partial derivatives $\left(\frac{\partial \Psi}{\partial \rho}\right)_{e,m}$ and $\left(\frac{\partial \Psi}{\partial e}\right)_{\rho,m}$ at a state point (ρ_1, e_1) in a subtable m are computed using the values of Ψ at the current state point and a second state point (ρ_2, e_2) in a very small interval. In Figures 3.3b and 3.3c the schematics of the perturbation of Ψ from a target state point 1 to a state point 2 (in a very small interval) are shown. By using the perturbation method, the partial derivatives in the subtable m are computed as follows

$$\left(\frac{\partial \Psi}{\partial \rho}\right)_{e,m} = \frac{\Psi_2^m|_{(\rho_2, e_1)} - \Psi_1^m|_{(\rho_1, e_1)}}{\delta \rho}, \quad \left(\frac{\partial \Psi}{\partial e}\right)_{\rho,m} = \frac{\Psi_2^m|_{(\rho_1, e_2)} - \Psi_1^m|_{(\rho_1, e_1)}}{\delta e}, \quad (3.4)$$

where $\delta \rho = \rho_2 - \rho_1$ and $\delta e = e_2 - e_1$ are the small intervals, which are defined along the constant e and constant ρ lines, respectively.

In order to compute the partial derivatives of Ψ in the overlap region between the subtables m and n , one may take the derivative of Ψ_{mn} in equation (3.2), which gives

$$\left(\frac{\partial \Psi}{\partial \rho}\right)_{e,mn} = -\frac{\Delta \Psi_{mn}}{\Delta \rho_{mn}^{ba}} + \beta \left(\frac{\partial \Psi}{\partial \rho}\right)_{e,m} + (1 - \beta) \left(\frac{\partial \Psi}{\partial \rho}\right)_{e,n}, \quad (3.5)$$

$$\left(\frac{\partial \Psi}{\partial e}\right)_{\rho,mn} = \beta \left(\frac{\partial \Psi}{\partial e}\right)_{\rho,m} + (1 - \beta) \left(\frac{\partial \Psi}{\partial e}\right)_{\rho,n}, \quad (3.6)$$

where $\Delta \rho_{mn}^{ba} = \rho_n^a - \rho_m^b$, and $\Delta \Psi_{mn} = \Psi_n - \Psi_m$. The partial derivatives in these equations can be computed either using the finite element approach or the perturbation method. Furthermore, the weight function β is computed at the current thermodynamic state. Therefore, the weight function in Figure 3.3b is with $\beta = \beta_1$, and in Figure 3.3c with $\beta = \beta_c$. Note that β_c in Figure 3.3c is constant. This is because $\rho = \rho_c$ is constant in the domain that is presented in this figure.

When using equation (3.5) for the pressure p in the overlap regions, the negative values of $\left(\frac{\partial p}{\partial \rho}\right)_{e,mn}$ must be avoided in order to prevent imaginary values for the speed of sound. This could occur only when we have $\frac{\Delta p_{mn}}{\Delta \rho_{mn}^{ba}} > 0$ with large enough values. Note that in the prepared tables we have $\Delta \rho_{mn}^{ba} < 0$. Furthermore, for the same value of ρ the values of p in the subtable n are never smaller than the values of p in the neighboring subtable m , and we have $\Delta p_{mn} \geq 0$. Therefore, for all the neighboring subtables we have $\frac{\Delta p_{mn}}{\Delta \rho_{mn}^{ba}} \leq 0$, which shows that $\left(\frac{\partial p}{\partial \rho}\right)_{e,mn}$ obtained from equation (3.5) is always positive.

3.2 Failure of the conventional look-up procedures

Several trial tables were prepared based on different data sizes with a total number of $n_\rho \times n_e$ data. The accuracy of the tables was determined as a function of the size of the tables. The accuracy is estimated by computing the maximum relative error of interpolations $\tilde{E}_{max}(u, u_{exact})_{cell}$ between the interpolated values u and the analytical values u_{exact} for a number of sample points in each cell, for which

$$\tilde{E}_{max}(u, u_{exact}) = \max(\tilde{E}(u_i, u_{exact,i})), \quad i = \{1, \dots, \mathcal{N}\}_{cell}. \quad (3.7)$$

Here, i is the index of the sample inspecting points in the cell, and $\mathcal{N} = [n_{e,cell} \times n_{\rho,cell}]$ is the total number of the inspecting points in each cell. Additionally, the relative error

Figure 3.4: Plots of the maximum relative error of interpolation $\tilde{E}_{max}$ (logarithmic scale), with the ranges of temperature $273.1 \leq T \leq 350$ K, dimensionless density $0.8818 \leq \eta \leq 0.8873$, and the corresponding values of the dimensionless internal energy ζ . $[n_e \times n_p] = [6001 \times 827]$ is the number of data points, and $[n_{e,cell} \times n_{p,cell}] = [50 \times 10]$ is the number of sample inspecting points, for (a) pressure, and (b) speed of sound.

function $\tilde{E}$ is defined in equation (2.36). For all of the trial tables, it was found that the global accuracy of the interpolations for pressure p and speed of sound c was much lower than that for temperature T . For instance, Figure 3.4 shows the maximum relative error of the interpolations $\tilde{E}_{max}$ for p and c in a part of a trial subtable. This figure is prepared for $[n_e \times n_p] = [6001 \times 827]$ data points in the table, and $[n_{e,cell} \times n_{p,cell}] = [50 \times 10]$ sample inspecting points in each cell. Furthermore, the dimensionless density η and the dimensionless internal energy ζ , which are defined at the beginning of this chapter, are used in these plots.

The figure shows that the accuracy of the interpolations for p and c is very low, that is, very high interpolation errors with $\{\tilde{E}_{max,p}, \tilde{E}_{max,c}\} = O(10^{-1})$. This behavior was observed in all the prepared subtables. Moreover, from Figure 3.4 it is visible that there are some overshoots in the relative error of interpolations for both p and c . These inaccuracies significantly reduce the global accuracy of the interpolations. It was found that the areas where these large inaccuracies occur coincide with cells containing multiphase data nodes, that is, phase-transitioning regions of the tables. For the uniform-phase (mixture/vapor/liquid) zones of the tables, the accuracy of the interpolations is much higher than the phase-transitioning regions and can become adequately accurate depending on the resolution of the data grid of the tables.

However, for the phase-transitioning regions, when using the conventional look-up methods, the accuracy of the interpolations is low, and rather insensitive to the resolution of the data grid. Therefore, refining the data grid in order to improve the accuracy of the interpolations in the multiphase tables is very inefficient and does not yield sufficiently accurate interpolated data. The failure of the conventional look-up procedures in multiphase thermodynamic tables is due to a nonsmooth distribution of the data in the phase-transitioning parts of these tables. A schematic representation of the actual distribution of the data (in particular $\Psi = \{p, c\}$) in a liquid-mixture transition cell

is depicted in Figure 3.5a. A slope-discontinuous distribution of the data around the saturation curve is visible in this figure. Additionally, a schematic of the interpolated data

Figure 3.5: Schematic of (a) the actual distribution of the data in a transition cell, and (b) the bilinear interpolations of the data in a transition cell.

in the transition cell using a conventional interpolation method (bilinear interpolation in this case) is shown in Figure 3.5b. A comparison of these figures explains the reason for the inaccuracy of the conventional look-up procedures.

Furthermore, one may consider using the interpolated data based on the transformed logarithmic form of the thermodynamic variables. However, compared to the non-logarithmic approach, the logarithmic variable interpolations did not improve the accuracy of the interpolations. The main reason for this is again the non-smooth behavior of the variables at the phase-transitioning regions of the tables. Note that the logarithmic transformations do not smooth out the variables. Therefore, the non-smooth parts also cause inaccuracies in the interpolated data based on the logarithmic variables. Moreover, any combination of the logarithmic grid spacing with the logarithmic variables interpolations was not found beneficial. The usage of the logarithmic transformations for the tables is thus not considered further in this thesis.

3.3 POITC

A Phase-Oriented Interpolations in (phase)-Transitioning Cells (POITC) method is developed in this section, for interpolating the data in the phase-transitioning zones of the multiphase thermodynamic tables ².

3.3.1 Procedure

A set of two-dimensional (ρ, e) -based multiphase tables is prepared for the thermodynamic variables $\Psi = \{T, p, c, \alpha\}$. The transition cells are identified in these tables by means of a flag. As seen in Figure 3.6a, within such a transition cell a linear approximation of the saturation curve is used. In the same figure, two saturation points (solid square symbols) are identified. The data in these saturation points, is also stored in the tables. In section 3.3.2 the procedure for characterizing these saturation points is described.

²Part of the contents of this section is based on Refs. [65] and [63]

Figure 3.6: Schematics of a phase-transitioning liquid-mixture cell for a multiphase table, with the data nodes in the mixture region (O), the liquid region (x), the saturation state (■), the sample state point (●), and the saturation curve (dotted curve); (a) approximating the saturation curve linearly; (b) triangulation of the transition cell.

The next steps explain the actual procedure for the interpolation of the data. A triangulation is generated in each transition cell, by subdividing the domain of the transition cell into a set $T_h = \{t_1, \dots, t_m\}$ of nonoverlapping triangles as presented in Figure 3.6b. The triangles are generated by setting the nodes of the transition cell as vertices of the triangles, and the saturation line included as a triangular edge. Note that other types of triangulations are needed for different locations of the solid squares (see Appendix D).

The domain for the interpolation of the data within the transition cell is now divided into smaller triangular domains, each triangle containing only uniform-phase data (with an approximation for the vicinity of the saturation curve). Knowing the location of a state point (ρ, e) in a transition cell, the triangle t_m containing this point needs to be identified for carrying out interpolations within that triangle. To handle this, properties of the barycentric coordinates are exploited that provide a simple algorithm for determining whether a point is inside a triangle or not (see Appendix E.1). Finally, the thermodynamic data is interpolated within the target triangle by carrying out a linear interpolation in barycentric coordinates (see Appendix E.2).

The interpolation of the speed of sound c using POITC is not performed directly, but using the mapped variable $\xi = \frac{1}{c^2}$ instead (see section 2.4.3). Figure 3.7 shows the plots of c and ξ in part of a subtable that includes phase-transitioning regions. It is observed that $\xi(\rho, e)$ is a smooth function compared to $c(\rho, e)$ itself. Therefore, the interpolation procedure is performed for ξ . After interpolating ξ using POITC, a reverse mapping is performed to obtain the value of the speed of sound $c = \frac{1}{\sqrt{\xi}}$ at this point. This step is necessary when implementing POITC for the speed of sound; without introduction of ξ the interpolations are not sufficiently accurate.

To assess the accuracy of POITC, the sample thermodynamic table used in the preceding section with conditions presented in Figure 3.4 is considered. In order to prepare the table, a smaller number of data points with $[n_e \times n_\rho] = [1101 \times 144]$ are used in this case compared to the previous example. The accuracy is assessed using $[n_{e,cell} \times n_{\rho,cell}] = [50 \times 10]$ sample state points in each transition cell. Additionally, around the saturation line a number of $n_{sat,cell} = 196$ randomly chosen sample thermodynamic state points (which could possess higher interpolation errors) are tested. A schematic of the sample state points in the transition cell is shown in Figure 3.8 (the number of the sample state points in this figure is arbitrary).

Figure 3.7: The speed of sound c and the mapped variable $\xi = \frac{1}{c^2}$ vs. the nondimensional density η and the nondimensional internal energy ζ . Here, $273.1 \leq T \leq 350$ K, and $0.8818 \leq \eta \leq 0.8873$, with the corresponding values of ζ .

Figure 3.8: Schematic of the sample state points (with an arbitrary number of the points) in a triangulated transition cell.

The accuracy study of the provided table, when using the POITC look-up procedure, is presented in Figure 3.9. It is evident that there is a significant improvement in the accuracy of the interpolations for the variables p and c when using the POITC approach (Figure 3.9) compared to the conventional method (Figure 3.4). A quantitative comparison of both methods for some tables with different sizes and with the same thermodynamic ranges is presented in Table 3.1. For the thermodynamic tables of the same size (cases 1 and 4 in Table 3.1), the one prepared based on the POITC approach (case 4) is 5 orders of magnitude more accurate than the one prepared based on the conventional approach (case 1). Even using a much larger number of data points does not quite improve the accuracy of the interpolated data when the conventional approach is employed. For instance, the accuracy of the conventional approach for case 3 is still 3 orders of magnitude lower than that of the POITC method for case 4, which is almost 40 times smaller in size than case 3.

Figure 3.10 shows part of a sample table that uses the POITC approach. For clarity, only the transition cells are shown in these figures. Figure 3.10a shows a plot of the saturation curve obtained using POITC for this sample table. An enlargement of a part of the plotted saturation curve is shown in Figure 3.10b. This plot demonstrates how the saturation curve is generated through the POITC approach, which is composed of a mesh of phase-transitioning cells. Moreover, the middle line passing through the transition cells

Figure 3.9: Maximum relative errors of POITC interpolation $\tilde{E}_{max}$ (logarithmic scale) for a table with the range of the temperature $273.1 \leq T \leq 350$ K, the dimensionless density $0.8818 \leq \eta \leq 0.8873$, and the corresponding values of the dimensionless internal energy ζ , and with $[n_e \times n_p] = [1101 \times 144]$ number of data points, by inspecting a number of $[n_{e,cell} \times n_{p,cell}, n_{sat,cell}] = [50 \times 10, 196]$ sample points, for (a) pressure, and (b) speed of sound.

Table 3.1: Comparison of the accuracy of POITC to the accuracy of conventional method of interpolation for some sample tables

Case	POITC	$\tilde{E}_{max,p}$	$\tilde{E}_{max,c}$	$n_e \times n_p$	MByte
1	No	10	10	1101×144	~ 1.2
2	No	1	10^{-1}	4001×552	~ 17
3	No	10^{-1}	10^{-1}	6001×827	~ 38
4	Yes	10^{-4}	10^{-4}	1101×144	~ 1.2

Note. The tables have been prepared for the ranges of dimensionless density $0.8818 \leq \eta \leq 0.8873$, temperatures of $273.1 \leq T \leq 350$ K, and the corresponding values of the dimensionless internal energy ζ . Errors are obtained by inspecting a number of $[n_{e,cell} \times n_{p,cell}, n_{sat,cell}] = [50 \times 10, 196]$ sample points in every cell.

in Figure 3.10b is the piecewise linear approximation of the saturation curve.

3.3.2 Characterization of the saturation points

Figure 3.11 shows a schematic of two sample types of the transition cell for water as well as their $p-v$ diagram. In order to characterize the saturation data points 5 and 6, the values of the independent variables ρ and e must be known at these points. From the transition cell in Figure 3.11a, it is evident that only one of the (ρ, e) variables is known

Figure 3.10: Part of a sample ρ - e table (only phase-transitioning cells are shown) constructed using POITC. The table is prepared based on ranges of the dimensionless density $0.9068 \leq \eta \leq 0.9118$, the temperature of $273.1 \leq T \leq 350$ K, and the corresponding values of the dimensionless internal energy ζ , and using $[n_e \times n_\rho] = [501 \times 66]$ data points; (a) saturation curve generated through a mesh of transition cells, and (b) magnified view: the mesh of transition cells showing different triangulations in each cell.

for each of the saturation points 5 and 6. In this case, the known variables are the density in point 5, that is, ρ_5 , and the internal energy in point 6, that is, e_6 , and the unknowns are e_5 and ρ_6 . For the transition cell in Figure 3.11b, the known variables are ρ_5 and ρ_6 and the unknowns are e_5 and e_6 . These unknowns can be computed by solving the employed thermodynamic relations.

Alternatively, a simple approach can be used without requiring the use of the thermodynamic relations. In this approach, the unknown variables ρ or e at points 5 and 6 can be determined using two auxiliary saturation points 7 and 8 (the open square symbols in Figure 3.11) on the saturation curve. These auxiliary points are along the constant-temperature lines in the p - v diagram that pass through one of the data nodes of the cell. Therefore, the thermodynamic state of the auxiliary points 7 and 8 can be determined based on the known data points $\{1, \dots, 4\}$. For the thermodynamic relations introduced in section 2.4.2 the variables in the saturation state are only a function of the temperature. Hence, the following differential relations can be written for the variables ρ and e in a saturation state:

$$\frac{de_{sat}(T)}{d\rho_{sat}(T)} = \frac{de_{sat}(T)}{dT} \frac{dT}{d\rho_{sat}(T)} = C_v \frac{dT}{d\rho_{sat}(T)}. \quad (3.8)$$

Here, in the second equality C_v is the specific heat at constant volume. Since the saturation curve in each transition cell is approximated linearly, equation (3.8) can be written in linearized form. For example, the relation between the values of the known auxiliary points 7 and 8 and the values of the saturation points 5 and 6 is given by

$$\frac{e_{sat,8} - e_{sat,5}}{\rho_{sat,8} - \rho_{sat,5}} = \frac{e_{sat,8} - e_{sat,6}}{\rho_{sat,8} - \rho_{sat,6}} = C_v \frac{T_8 - T_7}{\rho_{sat,8}(T_8) - \rho_{sat,7}(T_7)}. \quad (3.9)$$

Using equation (3.9), the unknown independent variable $\{\rho \text{ or } e\}$ at point 5 or 6 is interpolated/extrapolated along the approximated saturation line. It is noticed that the

Figure 3.11: Schematic of two types of the transition cell, and their corresponding $p - v$ diagram, with the data nodes in the mixture region (○), the liquid region (×), the saturation line (■), and with the auxiliary nodes on the saturation line (□); The dotted lines are iso-contours of constant temperature.

transition cell types shown in Figure 3.11 do not correspond to all types of the transition cells (see Appendix D). The above simplified approach is used in the numerical simulations described in this thesis.

3.3.3 Preparing the tables using POITC approach

Two-dimensional $\rho - e$ multiphase thermodynamic tables have been constructed in several split sub-domain regions, using the approaches that were described in preceding sections. Each subtable has an $n_\rho \times n_e$ number of data points. Moreover, each subtable has a grid cell size of $\Delta\rho \times \Delta e$, where

$$\Delta\rho = \frac{\rho_b - \rho_a}{n_\rho - 1}, \quad \Delta e = \frac{e_b - e_a}{n_e - 1}, \quad (3.10)$$

with indices a and b denoting the starting and the ending values of the variables ρ and e in each subtable, respectively. When preparing the tables, the values of n_ρ and n_e , and their Aspect Ratio

$$AR_{cell} := n_\rho / n_e, \quad (3.11)$$

need to be defined carefully, especially in the phase-transitioning regions; otherwise the tables will not provide sufficiently accurate interpolated data. The schematic view of

the multi-phase table that was presented in Figure 3.1a in section 3.1 shows that in the phase-transitioning regions the arrangement of transition cells is mostly staircase-like, but also some horizontally/vertically aligned transition cells are present as well. It has been observed that the interpolation in parts of the phase-transitioning cells with horizontally/vertically aligned cells are less accurate. Arrangement of the transition cells is dependent on the values of n_p , n_e , and on AR_{cell} . Hence, they have been defined such that the cell alignments are as much as possible staircase-type in the phase-transitioning regions, although almost in all the phase-transitioning regions the presence of some horizontal/vertical-type alignments could not be avoided.

The multi-phase thermodynamic tables have been prepared using 13 subtables. The nondimensional variables $\zeta = \frac{e}{e_\zeta}$ and $\eta = \frac{\rho}{\rho_\eta}$, with $\rho_\eta = 1100 \text{ kg m}^{-3}$ and $e_\zeta = 2.48433698 \times 10^6 \text{ J kg}^{-1}$, are used for the internal energy e and the density ρ , respectively. In Figure 3.12a a plot of the subtables in $\zeta - \eta$ space is presented (shown in logarithmic scale). This plots in this figure show the entire ranges of the dimensionless internal energy ζ and the entire ranges of the dimensionless density η for each subtable. Note that in each subtable there are some regions that are undefined (see section 3.1.1). In Figure 3.12b the defined ranges of the subtables are presented. The top (green) and bottom (red) lines in this figure are saturation/vapor and saturation/liquid states, respectively. The area between these lines is the mixture phase for which plots of the constant-density mixture curves are presented. These curves specify either a lower or a higher bound of the states in each subtable, which are plotted based on the prescribed ranges of the η and the corresponding values of ζ in that subtable. The overlapping parts between the neighboring regions are also visible. It is observed that the subtables with the density ranges of less than order of one possess much higher values for the energy compared to the regions with higher values of the density. Therefore, the bounding curves of regions with higher density values are not clearly visible in this figure. It is noticed that, the data that is stored in the thermodynamic tables is based on the ranges of the η and ζ variables shown in Figure 3.12a (which also include the regions with undefined states). However, the states that are not defined for the provided ranges of η and ζ are flagged as undefined within the subtables.

The data, which is used for preparing the thermodynamic tables, is shown in Table 3.2 and Table 3.3. All the subtables are prepared for temperature ranges of $273.1 \leq T \leq 350\text{K}$. In Table 3.2 the ranges of the dimensionless density η and the corresponding ranges of the dimensionless internal energy ζ in each subtable are presented. The thermodynamic tables are divided into subtables in terms of the density ranges. The upper and lower bounds of the density in each subtable are such that there is an overlap zone between every set of two subsequent neighboring subtables. For the given ranges of temperature and density in each region, the corresponding energy ranges are calculated using the provided thermodynamic relations (section 2.4.2). Table 3.3 contains the number of data points n_p and n_e , determined based on the derived accuracy of the POITC approach in the parts with phase-transitioning. Also, for each subtable, the interpolation method used, and the accuracy of the interpolation in each subtable is given. The maximum relative errors of interpolations for the pressure and the speed of sound, i.e., $\tilde{E}_{max,p}$ and $\tilde{E}_{max,c}$, respectively, were computed in each subtable using sample state points with $[n_{e,cell} \times n_{p,cell}] = [40 \times 20]$ for the uniform-phase cells and $[n_{e,cell} \times n_{p,cell}, n_{sat,cell}] = [50 \times 10, 196]$ for phase-transitioning cells. Additionally, the ranges of the thermodynamic subtables that contain the phase-transitioning regions are

(a)

(b)

Figure 3.12: Prepared thermodynamic table regions (with $N_{tot} = 13$ subtables): (a) $\zeta - \eta$ plot of the subtables in logarithmic scale showing the total ranges of ζ (including the regions with undefined states) for the ranges of η in each subtable. Note that the subtables 10 – 13 are not visible in this plot; (b) A $T - \zeta$ plot of the subtables showing the ranges of ζ (excluding the regions with undefined states) for the ranges of η in each subtable (the striped areas are the overlap regions). Note that subtables 1 – 7 are not visible in this plot.

determined by considering the ranges of the dimensionless density for the mixture-vapor zone with $4.3916 \times 10^{-6} \lesssim \eta_{mix-v} \lesssim 2.3627 \times 10^{-4}$ and $0.8852 \lesssim \eta_{mix-l} \lesssim 0.9089$.

The thermodynamic subtable No.1 contains the vapor-only data for which the interpolation has been performed using the non-POITC approach (a bilinear interpolation in the table cell). This region corresponds to the top green line in Figure 3.12b, which is

Table 3.2: Subtables of the constructed multiphase thermodynamic tables (13 subtables), the ranges of the dimensionless density η , and the corresponding dimensionless internal energy ζ for each subtable, obtained for the temperatures within $273.1 \leq T \leq 350\text{K}$

subtable	$[\eta_a, \eta_b]$	$[\zeta_a, \zeta_b]$
1	$[9.0909 \times 10^{-10}, 4.3636 \times 10^{-6}]$	$[0.9563, 1.0000]$
2	$[4.1818 \times 10^{-6}, 9.0909 \times 10^{-6}]$	$[0.4621, 0.9626]$
3	$[8.1818 \times 10^{-6}, 3.6364 \times 10^{-5}]$	$[0.1156, 0.9763]$
4	$[2.7273 \times 10^{-5}, 2.7273 \times 10^{-4}]$	$[0.0156, 1.0000]$
5	$[2.5455 \times 10^{-4}, 9.0909 \times 10^{-4}]$	$[0.0048, 0.9375]$
6	$[8.1818 \times 10^{-4}, 0.0045]$	$[0.0011, 0.3808]$
7	$[0.0036, 0.0182]$	$[3.9056 \times 10^{-4}, 0.1859]$
8	$[0.0145, 0.0909]$	$[2.0580 \times 10^{-4}, 0.1435]$
9	$[0.0727, 0.8182]$	$[1.6474 \times 10^{-4}, 0.1321]$
10	$[0.8045, 0.8836]$	$[1.6436 \times 10^{-4}, 0.12957]$
11	$[0.8818, 0.9073]$	$[1.6423 \times 10^{-4}, 0.129553]$
12	$[0.9068, 0.9118]$	$[1.6419 \times 10^{-4}, 0.129552]$
13	$[0.9109, 1.0000]$	$[1.6423 \times 10^{-4}, 0.129552]$

Note. Indices a and b are the starting and ending values in each subtable.

the vapor/saturation line. Knowing the minimum possible value for the density of water in the mixture-vapor zone i.e. $\eta_{min,mix-v} \approx 4.3916 \times 10^{-6}$, the upper bound of the density in subtable No.1 is selected such that for the provided range, only the vapor phase exists. Due to the linear relations for the thermal and caloric equations of state in the vapor phase (See section 2), an adequate accuracy of interpolation has been achieved using a rather small number of data points. Furthermore, the maximum relative error of interpolations for these variables is up to machine accuracy.

The thermodynamic table region No.13 contains liquid-only data for which the non-POITC (bilinear interpolation in the table cell) approach has been applied as well. This region corresponds to the bottom red line in Figure 3.12b, which represents the liquid/saturation line. It is known that the maximum possible value for the mixture density of water in mixture-liquid phase-transitioning zones is $\eta_{max,mix-l} \approx 0.9089$. Therefore, for the provided ranges of η in subtable No.13 only the liquid phase exists. Since there are no phase-transitioning regions in this part of the table, an adequate accuracy of interpolations is achieved with only a small number of data points.

Knowing the maximum possible value of the mixture density of water in the mixture-vapor phase-transitioning zones, i.e., $\eta_{max,mix-v} \approx 2.3627 \times 10^{-4}$, and the minimum possible value of the mixture density of water in mixture-liquid phase-transitioning zones, that is, $\eta_{min,mix-l} \approx 0.8852$, the density ranges of the mixture-only table regions are determined. The thermodynamic subtables No.5 - No.10 contain only mixture data,

Table 3.3: Subtables of the constructed multiphase thermodynamic tables, showing the number of data points n_p and n_e , the interpolation method, and the maximum relative error of interpolations $\tilde{E}_{max}$ for pressure and speed of sound

subtable	$n_p \times n_e$	POITC	$\tilde{E}_{max,p}$	$\tilde{E}_{max,c}$
1	200×10	no	10^{-16}	10^{-5}
2	50×3800	yes	10^{-3}	10^{-4}
3	60×4000	yes	10^{-3}	10^{-4}
4	150×4500	yes	10^{-3}	10^{-3}
5	500×400	no	10^{-4}	10^{-4}
6	400×300	no	10^{-4}	10^{-4}
7	200×500	no	10^{-5}	10^{-5}
8	200×600	no	10^{-5}	10^{-6}
9	400×200	no	10^{-4}	10^{-5}
10	300×200	no	10^{-5}	10^{-4}
11	1300×4500	yes	10^{-4}	10^{-4}
12	1200×4000	yes	10^{-3}	10^{-3}
13	300×200	no	10^{-4}	10^{-6}

Note. The sample points of the state are created with $[n_{e,cell} \times n_{p,cell}] = [40 \times 20]$ for uniform-phase cells (liquid/vapor/mixture) and $[n_{e,cell} \times n_{p,cell}, n_{sat,cell}] = [50 \times 10, 196]$ for phase-transitioning cells.

for which, again a bilinear interpolation of data (non-POITC approach) yields adequate accuracy of interpolation.

Finally, using the known values of the mixture density bounds, the density ranges of the phase-transitioning regions are determined. The thermodynamic table regions No.2 - No.4 contain vapor-mixture phase-transitioning data, and the regions No.11 - No.12 contain liquid-mixture phase-transitioning data. The interpolation within these subtables is carried out using the developed POITC approach. Due to the presence of the phase-transitioning cells in these regions, a relatively large number of data points was required to achieve adequate accuracy within these regions. Even using the POITC approach, achieving the desired accuracy in phase-transitioning regions still requires a higher resolution of data points compared to the single-state regions of the tables. The reasons for this are given below.

- Because of the approximation of the saturation curve by piecewise straight lines in the phase-transitioning cells, the interpolation is not exactly confined to a single-phase state.
- The order of magnitude of e in the vapor-mixture zones is rather high (requires a higher resolution for the grid of the data points).

- There is a consistency error for the pressure in the saturation vapor state, $p_{v,sat}$ (Figure 2.5).
- Within a transition cell in the liquid-mixture zone, the difference between the values of the pressure or the speed of sound for the cell nodes that are in the saturation phase compared to the ones in the liquid phase is rather high. This may decrease the accuracy of the interpolations for the pressure and speed of sound within the triangulated transition cells.

In the constructed tables, the data interpolations for the temperature T are performed through a bilinear interpolation within the table cell (conventional non-POITC approach). The global maximum relative error of interpolations for T in the prepared tables is generally low, at most $\tilde{E} = O(10^{-4})$. For the pressure p and the speed of sound c , the conventional approach is used in the uniform-phase zones, and the POITC approach is used in the phase-transitioning zones. The errors of the interpolations for these variables are at most $\tilde{E}_{max,p}, \tilde{E}_{max,c} = O(10^{-3})$. Note that, due to the values of the relative error of inconsistency for pressure in the saturation vapor states, with magnitudes of at most $\tilde{E}(p_v^{v,sat}, p_{mix}^{v,sat}) = O(10^{-3})$, as shown in Figure 2.5, locally the accuracy of the interpolations for p is limited in these parts of the tables.

Moreover, the values of the relative error of interpolations presented in Table 3.3 are the maximum values. For example, from Figure 3.9 it is visible that these maximum errors are present in a very small part of the tables and in the rest of the domain the accuracy is several orders of magnitude higher. Furthermore, in chapter 5 it will be shown that if these relatively large inaccuracies that occur only in a small part of the tables are not treated, then these errors are translated into large errors in the flow solution in the entire computational domain. The global accuracy of the tables is significantly improved by using the POITC approach compared to using the conventional approach. Furthermore, the tables occupy only about 400 MB of memory for data stored in double precision, whereas if the tables were prepared based on the conventional approaches they would require hundreds of gigabytes of memory, and yet the results would not be sufficiently accurate in the phase-transitioning regions. Although the global accuracy of the multiphase tables was increased significantly by using POITC, the global accuracy is still dictated by the local accuracy in phase-transitioning regions. One may achieve even higher global accuracies by refining the data grid or by refining the triangulation of the transition cells, in the areas with lower accuracy.

NUMERICAL METHOD

The numerical approaches used in this thesis to solve inviscid and viscous compressible flow problems are presented. First, the Reynolds Averaged Navier Stokes (RANS) equations are described. Then the turbulence model required to close the system of RANS equations is presented. Subsequently, the space and time discretization of the equations using a finite volume approach are described. Then, the higher-order accurate Weighted Essentially Non-Oscillatory (WENO) reconstruction scheme in multidimensions is described, followed by a presentation of the maximum principle- and positivity-preserving properties and a maximum principle-preserving WENO scheme. Finally, this chapter ends by introducing a novel positivity-preserving WENO scheme developed in one space dimension.

4.1 RANS equations

The Reynolds averaged form of the Navier Stokes equations (2.1) in integral conservation form is given by

$$\frac{\partial}{\partial t} \iiint_{\Omega} \mathbf{U} \, d\Omega + \iint_{\Gamma=\partial\Omega} \vec{\mathbf{F}}_j(\mathbf{U}) n_j \, d\Gamma = \iint_{\Gamma=\partial\Omega} \vec{\mathbf{F}}_j^v n_j \, d\Gamma. \quad (4.1)$$

Here, it is assumed that Ω is a bounded stationary polygon domain in R^3 with boundary $\partial\Omega$, the vector $\mathbf{U}$ denotes the vector of conservative variables which was defined in equation (2.2). The $\vec{\mathbf{F}}_j(\mathbf{U}) n_j$ term is the normal component of the inviscid flux vector, which in Cartesian coordinates can be written as follows

$$\vec{\mathbf{F}}_j(\mathbf{U}) n_j = \begin{bmatrix} \rho u_n \\ \rho u_n u_i + p n_i \\ \rho u_n H \end{bmatrix}, \quad (4.2)$$

where $u_n = u_j n_j$ is the velocity normal to the surface $\Gamma = \partial\Omega$. Moreover, the $\vec{\mathbf{F}}_j^v n_j$ term is the normal component of the viscous flux vector, given by

$$\vec{\mathbf{F}}_j^v n_j = \begin{bmatrix} 0 \\ \hat{\tau}_{ij} n_j \\ \hat{\tau}_{jk} u_k n_j - \hat{q}_{\kappa,j} n_j \end{bmatrix}, \quad (4.3)$$

where $\hat{\tau}_{ij}$ and $\hat{q}_{\kappa,j}$ are the components of the viscous stress tensor, and the heat flux vector, respectively, which can be written as

$$\hat{\tau}_{ij} = \mu_{tot} \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right], \quad (4.4)$$

and

$$\hat{q}_{\kappa,j} = -\mu_{tot}^* C_p \frac{\partial T}{\partial x_j}. \quad (4.5)$$

Here C_p is the specific heat at constant pressure, which is assumed to be constant for the liquid phase and vapor phase, and for the mixture phase it is computed as follows. In order to compute the transport properties in the mixture phase, an average value can be evaluated through a blending of the values for the liquid and vapor phases (see e.g. Yuan *et al.* [140], Bensow *et al.* [6], and Lagumbay [73]). The blending coefficient is frequently chosen to be the vapor void fraction α [6, 140]. In Lagumbay [73] the quantities per unit volume are blended using the vapor void fraction α and the quantities per unit mass are blended using the mass fraction of vapor $f_v = \frac{\rho_v}{\rho} \alpha$. In this thesis, the blending approach used by Lagumbay [73] is adopted.

For the specific heat C_p , which is a quantity per unit mass, the mixture value $C_p = C_{pm}$ is obtained via a blending of $C_p = C_{pl}$ and $C_p = C_{pv}$ for the liquid phase and vapor phase, respectively, using the mass fraction of vapor f_v , such that

$$C_{pm} = f_v C_{pv} + (1 - f_v) C_{pl}, \quad (4.6)$$

note that for the ratio of the specific heats γ , a similar formula must be used, i.e.

$$\gamma_{pm} = f_v \gamma_{pv} + (1 - f_v) \gamma_{pl}. \quad (4.7)$$

Moreover, μ_{tot} in equation (4.4) is the total viscosity, which is the sum of the laminar and turbulent components, i.e. μ and $\hat{\mu}$, respectively:

$$\mu_{tot} = \mu + \hat{\mu}. \quad (4.8)$$

This relation follows from the Boussinesq hypothesis [139], which offers a linear relation for the turbulent (Reynolds) stress $\hat{\tau}$ that is proportional to the gradient of the mean velocity field of the flow,

$$\hat{\tau}_{ij} = \hat{\mu} \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right]. \quad (4.9)$$

The turbulent or eddy viscosity $\hat{\mu}$ is computed from a turbulence model (see section 4.2). For most of the standard cases with air as the working fluid, the dynamic viscosity μ satisfies the Sutherland's law ([136]). However, for cavitating flow, which involves liquid, vapor, and mixture phases of water simultaneously, Sutherland's law is not valid. In this thesis the dynamic viscosity of liquid and vapor are taken constant. The dynamic viscosity of the mixture is obtained from a blending of the liquid and vapor viscosities using the vapor void fraction α , given by

$$\mu_{mix} = \alpha \mu_v + (1 - \alpha) \mu_l. \quad (4.10)$$

Furthermore, for the heat flux, μ_{tot}^* is defined by

$$\mu_{tot}^* = \frac{\mu}{Pr} + \frac{\hat{\mu}}{\hat{Pr}}, \quad (4.11)$$

where Pr and $\hat{Pr}$ are the molecular and turbulent Prandtl numbers, respectively. For cavitating flows, it is assumed that the molecular and turbulent Prandtl numbers for liquid and vapor are constant. The mixture values of the Prandtl number is defined as follows. Since $Pr = \frac{C_p \mu}{\kappa}$, with κ the thermal conductivity, knowing the mixture values of C_p , μ , and κ the value of the mixture Pr can be computed. The procedures for computing the mixture values of C_p and μ are already described. The mixture value of κ is computed from

$$\kappa_{mix} = \alpha \kappa_v + (1 - \alpha) \kappa_l, \quad (4.12)$$

where, κ_l and κ_v are the liquid and vapor thermal conductivities, respectively.

4.2 Turbulence modeling

The definition of the molecular (or dynamic) and turbulent viscosities was presented in the preceding section. The turbulent viscosity is computed from a turbulence model. In this thesis, the Spalart-Allmaras (S-A) and Menter Shear Stress Transport (SST) models are employed, which are described in the following.

S-A model

The one-equation S-A model uses a transport equation for a variable $\hat{\nu}$ which is directly related to the eddy-viscosity $\hat{\mu}$ by the following relation

$$\hat{\mu} = \rho \hat{\nu} f_{v1}, \quad f_{v1} = \frac{\mathcal{X}^3}{\mathcal{X}^3 + C_{v1}^3}, \quad \mathcal{X} = \frac{\hat{\nu}}{\nu}, \quad \nu = \frac{\mu}{\rho}. \quad (4.13)$$

The transport equation for $\hat{\nu}$ can be written as follows

$$\frac{\partial \hat{\nu}}{\partial t} + \frac{\partial}{\partial x_j} (\hat{\nu} u_j) - \frac{\partial}{\partial x_j} \left(\frac{(\nu + \hat{\nu})}{\sigma} \frac{\partial \hat{\nu}}{\partial x_j} \right) = C_{b1} \hat{S} \hat{\nu} + \frac{C_{b2}}{\sigma} \left(\frac{\partial \hat{\nu}}{\partial x_j} \right)^2 - C_{w1} f_w \left(\frac{\hat{\nu}}{d_S} \right)^2, \quad (4.14)$$

where $\nu = \frac{\mu}{\rho}$ is the (molecular) kinematic viscosity, and d_S is the distance to the nearest wall. The production term $\hat{S}$ is defined as $\hat{S} = |\tilde{\omega}| + \frac{\hat{\nu}}{\kappa^2 d_S^2} f_{v2}$, $|\tilde{\omega}| = \sqrt{\tilde{\omega}_i \tilde{\omega}_i}$ is the magnitude of the fluid vorticity vector with $\tilde{\omega}_i = \epsilon_{ijk} \frac{\partial u_k}{\partial x_j}$ (ϵ_{ijk} is the Levi-Civita tensor), and $f_{v2} = 1 - \frac{\mathcal{X}}{1 + \mathcal{X} f_{v1}}$. The function f_w is defined by $f_w = g \left[\frac{1 + C_{w3}^6}{g^6 + C_{w3}^6} \right]^{1/6}$ with $g = r + C_{w2} (r^6 - r)$ and $r = \frac{\hat{\nu}}{\hat{S} \kappa^2 d_S^2}$. Furthermore, the constants in the model are

$$\sigma = \frac{2}{3}, \quad C_{b1} = 0.1355, \quad C_{b2} = 0.622, \quad \kappa = 0.41, \quad C_{w1} = \frac{C_{b1}}{\kappa^2} + \frac{1 + C_{b2}}{\sigma}, \quad C_{w2} = 0.3, \quad C_{w3} = 2, \quad C_{v1} = 7.1. \quad (4.15)$$

Menter SST Model

The Menter SST turbulence model (Menter [89]) is a two-equation model for the turbulent kinetic energy $\hat{k}$ and specific dissipation $\hat{\omega}$. The SST model blends the $k - \omega$ and $k - \varepsilon$ models, and it is formulated as a $k - \omega$ model with transported conserved variables

$$\hat{\mathbf{U}} = [\rho\hat{k}, \rho\hat{\omega}]^T. \quad (4.16)$$

The eddy viscosity $\hat{\mu}$ is computed using the variables in $\hat{\mathbf{U}}$ as follows

$$\hat{\mu} = \frac{\rho a_1 \hat{k}}{\max(a_1 \hat{\omega}, S F_2)}, \quad (4.17)$$

where $S = \sqrt{2S_{ij}S_{ij}}$, with $S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ denoting the component of strain rate tensor, and F_2 is the second blending function [89].

The SST transport equations for the components of $\hat{\mathbf{U}}$ can be written as follows

$$\frac{\partial(\rho\hat{k})}{\partial t} + \frac{\partial(\rho u_j \hat{k})}{\partial x_j} = P_{\hat{k}} - \beta^* \rho \hat{k} \hat{\omega} + \frac{\partial}{\partial x_j} \left((\mu + \sigma_k \hat{\mu}) \frac{\partial \hat{k}}{\partial x_j} \right), \quad (4.18)$$

$$\begin{aligned} \frac{\partial(\rho\hat{\omega})}{\partial t} + \frac{\partial(\rho u_j \hat{\omega})}{\partial x_j} &= \frac{\gamma}{\hat{\nu}} P_{\hat{k}} - \beta \rho \hat{\omega}^2 + \frac{\partial}{\partial x_j} \left((\mu + \sigma_\omega \hat{\mu}) \frac{\partial \hat{\omega}}{\partial x_j} \right) \\ &\quad + 2(1 - F_1) \frac{\rho \sigma_{\omega 2}}{\hat{\omega}} \frac{\partial \hat{k}}{\partial x_j} \frac{\partial \hat{\omega}}{\partial x_j}, \end{aligned} \quad (4.19)$$

where

$$P_{\hat{k}} = \hat{\tau}_{ij} \frac{\partial u_i}{\partial x_j}, \quad (4.20)$$

is the production of turbulent kinetic energy, with turbulent stress tensor $\hat{\tau}_{ij}$ defined in equation (4.9). Furthermore, F_1 is the first blending function, and the value of the constants and the blending functions can be found in Menter [89], Menter *et al.* [90], and Rumsey [105].

4.3 Finite volume scheme

The computational domain is formed by a set of non-overlapping non-deforming cells V_k (k denotes the index of the grid cell) and with boundary ∂V_k which are assumed to cover Ω exactly. Both unstructured and structured (uniform or nonuniform) grids are used in this thesis, and it is assumed that each set of neighboring cells k and l share a complete edge/surface denoted by S_{kl} , i.e. hanging nodes are not allowed. For example, Figure 4.1 shows a uniform 1D grid with the cell centers $k + i$, $\{i = -1, \dots, 2\}$, and with the cell faces $k + i + 1/2$. Based on this assumption, the discretization of equation (4.1) using a cell-centered upwind finite volume formulation is described in the following.

Figure 4.1: Schematic of a 1D grid stencil consisting of four neighboring cells $k + i$, $\{i = -1, \dots, 2\}$, and with the cell faces $k + i + 1/2$. For example, cell k with faces $k - 1/2$ and $k + 1/2$ which are shared with the neighboring cells $k - 1$ and $k + 1$, respectively.

The semi-discretized form of equation (4.1) for each cell V_k in space can be written as

$$\frac{d\bar{\mathbf{U}}_k}{dt} = \mathfrak{R}_k := \mathfrak{R}_k^c + \mathfrak{R}_k^v, \quad (4.21)$$

where

$$\bar{\mathbf{U}}_k = \frac{1}{|V_k|} \iiint_{V_k} \mathbf{U} d\Omega_k, \quad (4.22)$$

is the cell averaged vector of conservative variables, and $\mathfrak{R}_k$ is the sum of the convective and viscous residuals, i.e. $\mathfrak{R}_k^c$ and $\mathfrak{R}_k^v$, respectively.

By replacing the inter-cell inviscid and viscous fluxes by numerical fluxes, and using the midpoint rule for the surface integrals, the residuals can be written as follows:

$$\mathfrak{R}_k^c = -\frac{1}{|V_k|} \sum_{l=1}^{N_{S,k}} \mathbf{H}(\mathbf{U}_{kl}^-, \mathbf{U}_{kl}^+, \mathbf{n}_{kl}) |\mathbf{S}_{kl}|, \quad (4.23)$$

and

$$\mathfrak{R}_k^v = \frac{1}{|V_k|} \sum_{l=1}^{N_{S,k}} \mathbf{H}^v |\mathbf{S}_{kl}|. \quad (4.24)$$

Here $\mathbf{n}_{kl}$ is the normalized vector of the face vector $\mathbf{S}_{kl}$, and $\mathbf{H}$ and $\mathbf{H}^v$ are the vectors of the inviscid and viscous numerical fluxes, which are discussed later on. Additionally, $(\cdot)_{kl}^-$ and $(\cdot)_{kl}^+$ denote the left and right state of the cell face S_{kl} , respectively.

In order to compute $\mathbf{H}(\mathbf{U}_{kl}^-, \mathbf{U}_{kl}^+)$, the values of $\mathbf{U}_{kl}^-$ and $\mathbf{U}_{kl}^+$ which are the approximations of the conserved variables on the left and right states of the cell face, respectively, must be known. Since at each time level, only the averaged value of the variables within each cell V_k are updated, the face values are unknown. However, the face values can be reconstructed using the values of the cell averages. Some of the most common reconstruction schemes are described in the following.

The most trivial choice for computation of $\mathbf{U}_{kl}^-$ and $\mathbf{U}_{kl}^+$ is to perform a constant reconstruction of the cell averages $\bar{\mathbf{U}}_k$ and $\bar{\mathbf{U}}_l$ on the faces, such that $\mathbf{U}_{kl}^- = \bar{\mathbf{U}}_k$ and $\mathbf{U}_{kl}^+ = \bar{\mathbf{U}}_l$. However, the constant reconstruction scheme is only first-order accurate, which is known to be much too dissipative numerically. The numerical dissipation is highly undesirable for solving problems with vortex cavitation. Therefore, higher-order accurate schemes are considered.

Second-order accurate schemes such as Monotonic Upstream-centered Schemes for Conservation Laws (MUSCL) of van Leer [130] (section 4.3.5), are less dissipative than the first-order schemes. However, in chapter 5 it is shown that when using the MUSCL schemes for solving the vortex cavitation problem the amount of the numerical dissipation

is still high, and an impractically high resolution of the spacial grid (in combination with extremely small time steps for resolving the flow physics) would thus be needed.

Alternatively, higher-order accurate (higher than second order) Weighted Essentially Non-Oscillatory (WENO) schemes are considered (section 4.4). The amount of the numerical dissipation in WENO schemes is rather low (negligible). Therefore, it appears that compared to the MUSCL schemes, the WENO schemes are much better suited for solving the vortex cavitation problems. The drawback of the WENO schemes is that they are not strictly monotonic, which can result in non-physical values of the flow variables. In order to avoid such problems, the scheme must obey a maximum principle (see section 4.5). A higher-order accurate shock-capturing scheme that obeys the maximum principle by its nature, i.e. without using limiter functions or any other special treatment, have never been developed. For the WENO scheme special treatments are used to enforce the maximum principle-preserving property. Some of the recently developed maximum principle-preserving WENO schemes, including a novel approach developed in this thesis, are discussed in section 4.5.

4.3.1 Inviscid numerical fluxes

Once the face values $\mathbf{U}_{kl}^-$ and $\mathbf{U}_{kl}^+$ on a face kl are known, the numerical fluxes can be computed. Due to presence of a non-smooth solution field in our numerical simulations, the numerical flux $\mathbf{H}(\cdot, \cdot)$ must be computed using an exact or approximate Riemann solver (see e.g. Toro [126]). In the current thesis we only consider the approximate Riemann solvers, because the exact solution involves iterative algorithms which can be computationally expensive.

One essential requirement for the numerical scheme for computation of the flux function $\mathbf{H}(\cdot, \cdot)$ is that it should be convergent (see e.g. [76]). This requires two conditions, consistency and stability. The method must be consistent with the differential equation, meaning that it approximates the differential equation well locally. This means that the truncation error tends to zero with decreasing spatial and temporal step sizes. In particular, $\mathbf{H}(\cdot, \cdot)$ must be a Lipschitz continuous function of its arguments. Furthermore, the flux function must be consistent with the physical flux $\vec{\mathbf{F}}_j(\mathbf{U})$ in equation (4.1), such that, given neighboring cells averages $\{\bar{\mathbf{U}}_{k-1}, \bar{\mathbf{U}}_k\}$ and for any vector $\tilde{\mathbf{U}}$, when $\bar{\mathbf{U}}_{k-1}, \bar{\mathbf{U}}_k \rightarrow \tilde{\mathbf{U}}$ we have $\mathbf{H}(\bar{\mathbf{U}}_{k-1}, \bar{\mathbf{U}}_k, \mathbf{n}) = \vec{\mathbf{F}}(\tilde{\mathbf{U}}) \cdot \mathbf{n}$. For the stability reasons, we need the function $\mathbf{H}(\cdot, \cdot)$ to be monotonic, i.e. nondecreasing in its first argument and nonincreasing in its second argument or symbolically we would have $\mathbf{H}(\uparrow, \downarrow)$. Furthermore, the flux function must be conservative such that, given the cell averages $\bar{\mathbf{U}}_k$ and $\bar{\mathbf{V}}_k$, we would have $\mathbf{H}(\bar{\mathbf{U}}_k, \bar{\mathbf{V}}_k, \mathbf{n}) = -\mathbf{H}(\bar{\mathbf{V}}_k, \bar{\mathbf{U}}_k, -\mathbf{n})$.

Conventional flux schemes such as the scheme of Jameson-Schmidt-Turkel (JST) [57] and classical Riemann solvers such as the Lax-Friedrichs scheme (see e.g. [77]) fail to solve the cavitation problem using a compressible flow approach. One of the reasons for this is that the classical flux schemes are not strictly monotonic (stability issue). Moreover, when a compressible flow model of cavitation is employed, the classical Riemann solvers are not sufficiently accurate and efficient for solving the liquid (incompressible) part of the cavitating flows using the compressible flow approach. These issues are discussed on the following.

In cavitating flows there are large jumps in the flow field variables, in particular the density (see e.g. Koop [68] for more details) and pressure. For example, at a temperature

of $T = 293 \text{ K}$ the saturated liquid and vapor densities are equal to $\rho_{l,sat} = 998.19 \text{ kg m}^{-3}$ and $\rho_{v,sat} = 0.0172 \text{ kg m}^{-3}$, respectively, resulting in a density ratio $\frac{\rho_{l,sat}}{\rho_{v,sat}} \approx 58000$. When using the JST flux scheme [57], near discontinuities such high ratios of the flow field variables cause relatively large over- and undershoots resulting in non-physical values, which significantly decrease the accuracy of the results and in most cases cause a failure of the numerical algorithm.

Moreover, the value of the speed of sound c in cavitating flows ranges from rather low values (e.g. with $c < 1 \text{ m s}^{-1}$) in the mixture to high values in the liquid (e.g. $c \approx 1500 \text{ m s}^{-1}$). Hence, the Mach number also ranges from low values in the liquid (low-Mach number flow) to relatively high values in the mixture. The solution from the classical Riemann solvers (which are originally designed to solve compressible flows) for low-Mach (incompressible) flows is incorrect. Liou [78] and Schmidt *et al.* [113] showed that this is because for the classical Riemann solvers the dissipation in the numerical approximations of the pressure for compressible flows is scaled by a term of $O(\rho c \Delta u)$ (dynamic waves), whereas the changes in pressure due to smooth changes in the flow scale with $O(\rho u \Delta u)$ (continuity waves). For the mixture phase at standard conditions ρc is of $O(10^2)$ and for water ρc is of $O(10^6)$. This shows that, when using the classical Riemann solvers, the dissipation effects for the calculation of the low Mach number (liquid water) flow becomes much higher than the ones for the mixture and the ones for the vapor.

To scale the acoustic wave speeds correctly for problems containing low-Mach number flows, preconditioning methods are used (see e.g. Chorin [17], Turkel [128], etc). Furthermore, the numerical methods for low-Mach number flows [40, 41] can be improved by modifying the flux schemes by a proper scaling of the numerical dissipation. An example of such a modified scheme is the flux-vector splitting scheme of Advection Upstream Splitting Method (AUSM) introduced by Liou & Steffen [80]). The AUSM scheme splits the flux-vector into two parts, namely, the convective flux and the pressure flux. First an interface Mach number at the cell face is computed using the characteristic speeds of the neighboring cells. The interface Mach number is then utilized to compute an upwind interpolation for the convective part of the inviscid fluxes. A separate Mach number splitting is used for computing the pressure terms. The later versions of AUSM, i.e. AUSM+ and AUSM+-up schemes ([78]) use a generalized Mach number based on convection and pressure splitting functions. Furthermore, an all-speed version of AUSM+-up based on low-Mach preconditioning was developed in [79]. The AUSM+ scheme has several desirable properties: it provides exact resolution of contact and shock discontinuities; it preserves positivity of scalar quantities (monotonicity); it results in oscillation-free numerical solutions near stationary and moving shocks (monotonicity and stability). In addition, Schmidt *et al.* [113] introduced a hybrid scheme based on the scheme of Harten-Lax-van Leer (HLLC) [127] and the AUSM scheme using a modified pressure flux formulation. The hybrid HLLC-AUSM scheme was utilized by Schmidt *et al.* [113] and Koop & Hoeijmakers [67] for the numerical simulation of cavitating flows.

We mainly use the AUSM+-up for all speeds (Liou [79]) flux scheme. This scheme showed rather good stability and accuracy in the numerical simulations of cavitating flows in this thesis. In addition, for some numerical experiments the hybrid HLLC-AUSM scheme is used (for description of the method see e.g. [113]).

4.3.2 AUSM+-up for all speeds scheme

The AUSM family of schemes for computing the inviscid numerical fluxes were discussed in the preceding subsection. In this subsection, the AUSM+-up for all speeds (Liou [79]) flux scheme is described. The AUSM scheme splits the inviscid flux $\mathbf{H}$ in two parts: a numerical convective flux $\mathbf{H}^{(c)}$ and a numerical pressure flux $\mathbf{H}^{(p)}$, such that at a cell face kl we can write:

$$\mathbf{H}(\mathbf{U}_{kl}^-, \mathbf{U}_{kl}^+, \mathbf{n}_{kl}) = \mathbf{H}^{(c)}(\mathbf{U}_{kl}^-, \mathbf{U}_{kl}^+, \mathbf{n}_{kl}) + \mathbf{H}^{(p)}(\mathbf{U}_{kl}^-, \mathbf{U}_{kl}^+, \mathbf{n}_{kl}). \quad (4.25)$$

The numerical convective flux $\mathbf{H}^{(c)}$ is defined in an upwind form as follows:

$$\mathbf{H}^{(c)}(\mathbf{U}_{kl}^-, \mathbf{U}_{kl}^+, \mathbf{n}_{kl}) = \bar{c} \bar{M} \rho_{kl}^\pm \phi_{kl}^\pm, \quad (4.26)$$

where $\bar{c} = \frac{1}{2}(c_{kl}^+ + c_{kl}^-)$ is the average speed of sound, $\phi = [1, \mathbf{u}^T, H]^T$, and we define

$$(\cdot)_{kl}^\pm = \begin{cases} (\cdot)_{kl}^- & \text{if } \bar{M} \geq 0 \\ (\cdot)_{kl}^+ & \text{if } \bar{M} < 0 \end{cases}. \quad (4.27)$$

$\bar{M}$ is the interface Mach number which is defined by

$$\bar{M} = \mathcal{M}_+^{(4)}(M_{kl}^-) + \mathcal{M}_-^{(4)}(M_{kl}^+) + \bar{M}_p, \quad (4.28)$$

where $\mathcal{M}_\pm^{(4)}$ are the polynomials which are defined in equation (4.38), and $\bar{M}_p$ is given by

$$\bar{M}_p = -\frac{K_p}{f_a} \max(1 - \sigma \tilde{M}^2, 0) \frac{p_{kl}^+ - p_{kl}^-}{\bar{\rho} \bar{c}^2}, \quad (4.29)$$

where,

$$\bar{\rho} = \frac{1}{2}(\rho_{kl}^- + \rho_{kl}^+), \quad \tilde{M}^2 = \frac{1}{2}((M_{kl}^-)^2 + (M_{kl}^+)^2), \quad (4.30)$$

and

$$f_a(M_0) = M_0(2 - M_0), \quad (4.31)$$

with

$$M_0 = \min(1, \max(\tilde{M}^2, M_{co}^2)). \quad (4.32)$$

Here $\sigma = 1.0$, $K_p = \frac{1}{4}$, and M_{co} is the cut-off Mach number which typically has a value of $M_{co} = \kappa_M M_\infty$, where $\kappa_M = O(1)$.

The numerical pressure flux $\mathbf{H}^{(p)}$ is defined as follows:

$$\mathbf{H}^{(p)}(\mathbf{U}_{kl}^-, \mathbf{U}_{kl}^+, \mathbf{n}_{kl}) = \bar{p} \begin{bmatrix} 0 \\ \mathbf{n}_{kl} \\ 0 \end{bmatrix}, \quad (4.33)$$

where, $\bar{p}$ is given by:

$$\bar{p} = p_{kl}^- \mathcal{P}_+^{(5)}(M_{kl}^-) + p_{kl}^+ \mathcal{P}_-^{(5)}(M_{kl}^+) + \bar{P}_u, \quad (4.34)$$

Here, $\mathcal{P}_{\pm}^{(5)}$ are the polynomials which are defined in equation (4.39), and

$$\bar{P}_u = -2f_a K_u \bar{\rho} \bar{c}^2 \mathcal{P}_+^{(5)}(M_{kl}^-) \mathcal{P}_-^{(5)}(M_{kl}^+) (M_{kl}^+ - M_{kl}^-), \quad (4.35)$$

with $K_u = \frac{3}{4}$.

The polynomial functions, which are required for computing $\bar{M}$ and $\bar{\rho}$, are defined as follows:

$$\mathcal{M}_{\pm}^{(1)}(M) = \frac{1}{2}(M \pm |M|), \quad (4.36)$$

$$\mathcal{M}_{\pm}^{(2)}(M) = \pm \frac{1}{4}(M \pm 1)^2, \quad (4.37)$$

$$\mathcal{M}_{\pm}^{(4)}(M) = \begin{cases} \mathcal{M}_{\pm}^{(1)}(M) & \text{if } |M| \geq 1 \\ \mathcal{M}_{\pm}^{(2)}(M) \left(1 \mp 16\beta \mathcal{M}_{\mp}^{(2)}(M)\right) & \text{if } |M| < 1 \end{cases}, \quad (4.38)$$

$$\mathcal{P}_{\pm}^{(5)}(M) = \begin{cases} \frac{1}{M} \mathcal{M}_{\pm}^{(1)}(M) & \text{if } |M| \geq 1 \\ \mathcal{M}_{\pm}^{(2)}(M) \left((\pm 2 - M) \mp 16\alpha M \mathcal{M}_{\mp}^{(2)}(M)\right) & \text{if } |M| < 1 \end{cases}, \quad (4.39)$$

where, $\beta = \frac{1}{8}$, $\alpha = \frac{3}{16}(-4 + 5f_a^2)$, and M must be replaced by M_{kl}^- or M_{kl}^+ , which are given by

$$M_{kl}^- = \frac{\mathbf{u}_{kl}^- \cdot \mathbf{n}}{\bar{c}}, \quad M_{kl}^+ = \frac{\mathbf{u}_{kl}^+ \cdot \mathbf{n}}{\bar{c}}. \quad (4.40)$$

4.3.3 Viscous numerical fluxes

In order to compute the viscous numerical fluxes $\mathbf{H}^v$ in 4.24 the procedure in [95] is adopted. The viscous fluxes are evaluated using the values of the flow quantities and their gradients at the cell faces. Furthermore, the value of the field variables including the velocity components u_j , the dynamic viscosity $\hat{\mu}$, and the heat conduction coefficient κ is averaged over each cell face.

The gradients of the flow variables are computed using the Gauss method over the cell centers. The Gauss theorem applied to the vector of cell averaged velocities $\bar{\mathbf{u}}$ within a cell V_k , in component form gives:

$$\iiint_{V_k} \frac{\partial u_i}{\partial x_j} d\Omega_k = \iint_{\Gamma=\partial\Omega} u_i n_j d\Gamma, \quad (4.41)$$

An approximate form of equation (4.41) can be used in order to compute the gradients $\left(\frac{\partial u_i}{\partial x_j}\right)_k$ at the cell V_k as follows:

$$\left(\frac{\partial u_i}{\partial x_j}\right)_k \approx \frac{1}{|V_k|} \sum_{l=1}^{N_{S,k}} \frac{1}{2} (u_{i,k} + u_{i,l}) n_{j,kl} |\mathbf{S}_{kl}|, \quad (4.42)$$

where $n_{j,kl}$ is the component of the normal vector on face kl , and k and l denote the indices of the neighboring cells V_k and V_l . The resulting gradients are then averaged to

obtain the gradients at the cell faces kl . In [95] an additional correction [135] step is applied in order to reduce the truncation error of the scheme and to avoid the odd-even decoupling problem. Using this correction term, the final expression for the gradients in the direction of $\mathbf{n}_{kl}$ can be written as follows:

$$\left(\frac{\partial u_i}{\partial x_j}\right)_{kl} n_{j,kl} = \frac{u_{i,l} - u_{i,k}}{|\mathbf{x}_l - \mathbf{x}_k|} \alpha_f + \frac{1}{2} \left(\left(\frac{\partial u_i}{\partial x_j}\right)_k + \left(\frac{\partial u_i}{\partial x_j}\right)_l \right) (n_{j,kl} - \alpha_f s_{j,f}), \quad (4.43)$$

where $s_{j,f}$ is the j -th component of the normalized vector connecting the cell centroids across the face, $|\mathbf{x}_l - \mathbf{x}_k|$ is the distance between the cell centroids of V_k and V_l and the coefficient α_f is defined by $\alpha_f = s_{j,f} n_{j,kl}$.

4.3.4 Boundary conditions

Far field

When considering the inlet and outlet boundaries for hyperbolic equations, the characteristic properties of the flow must be considered. The number of the physical boundary conditions for an unsteady problem depends on the characteristic properties of the flow, which may vary with position on the boundary or may change in time. A review of different approaches for treating such boundary conditions can be found in Colonius [19]. In the present thesis, the inflow and outflow boundary conditions are specified using a far field approach. The far field boundary is placed sufficiently far from the main computational domain, where also the resolution of the employed grid is taken several orders of magnitude coarser than that finest grid near the domain of interest. All halo cells in the far field (whether on inflow or outflow boundary) are set to the far field (or free-stream flow) conditions.

Specifying conditions at the outflow boundaries appears to be an overspecification of the boundary conditions which contradicts the well-posedness of the problem. However, at the outflow boundaries only the information from the inner domain is used. This can be checked by writing the Lax-Friedrichs flux scheme for a 1D unsteady transport equation (with a constant convection speed). The resulting expression only depends on the information at the left state of the interface. Therefore, at the outlet boundaries in the far field, where it is assumed that the information is transported with the speed of flow (with negligible flow disturbances), only the information at the left state of the boundary interface, i.e. the internal cells, is required, at least for a linear transport equation.

Solid wall in inviscid flow

For the solid walls in inviscid flow, a slip boundary condition is imposed. In this case, the numerical flux function $\mathbf{H}(\mathbf{U}_{kh,k}, \mathbf{U}_{kh,h})$ in equation (4.23) must be computed, in which $\mathbf{U}_{kh,k}$ and $\mathbf{U}_{kh,h}$ denote the values of the variables at the solid wall cell face kh on the side of the internal cell k and halo cell h , respectively. The halo cell values $\mathbf{U}_{kh,h}$ are evaluated using a symmetric boundary condition technique (see e.g. Blazek [9]). When using a non-permeability condition and the solid wall symmetry technique, neglecting the

effect of the curvature of the surface, the following gradients need to vanish:

$$\mathbf{n} \cdot \mathbf{u} = \mathbf{n} \cdot \nabla \rho = \mathbf{n} \cdot \nabla p = \mathbf{n} \cdot (\mathbf{u} - (\mathbf{n} \cdot \mathbf{u}) \mathbf{n}) = 0. \quad (4.44)$$

When the conditions in equation (4.44) are satisfied, the values in the halo cell are obtained. The halo cell values of the scalar quantities such as pressure and density are the reflected internal cell values. The vector quantities such as the velocities vector in the halo cells are the reflected internal velocities vector (with a change in sign of the face normal component). Therefore, given the values of the cell averages $\bar{\mathbf{U}}_{k_n} = [\rho_{k_n}, \mathbf{u}_{k_n}^T, p_{k_n}]^T$ with k_n denoting the index of the internal cells incrementing in the wall normal direction, the halo cell values $\bar{\mathbf{U}}_{h_n} = [\rho_{h_n}, \mathbf{u}_{h_n}^T, p_{h_n}]^T$ with h_n denoting the index of the halo cells incrementing in the reverse direction of the wall normal, are the following:

$$\rho_{h_n} = \rho_{k_n}, \quad p_{h_n} = p_{k_n}, \quad \mathbf{u}_{h_n} = \mathbf{u}_{k_n} - 2(\mathbf{u}_{k_n} \cdot \mathbf{n}) \mathbf{n}, \quad (4.45)$$

and the values of the higher indices are obtained using a similar approach. For example, the values of $\bar{\mathbf{U}}_{h_n+1}$ are obtained through replacement of the values of $\bar{\mathbf{U}}_{k_n}$ by $\bar{\mathbf{U}}_{k_n+1}$ in equation (4.45).

Moreover, an improved wall boundary conditions technique considering the effect of the curvature of the solid surface can be used (see e.g. Rizzi [103]), for which a pressure gradient function (dependent on the curvature) is implemented in the wall normal direction. The curvature corrected symmetry technique is not considered in the current thesis.

Solid wall in viscous flow

On a solid wall in viscous flow, the no-slip condition is applied by setting $\mathbf{u}_{wall} = 0$. Moreover, at a no-slip wall the eddy-viscosity should be equal to zero. When using the S-A model, this condition can be satisfied by directly setting $\hat{\nu} = 0$ in equation (4.13). When using the Menter SST model the eddy viscosity is obtained from equation (4.17). In order to get a zero eddy viscosity on a no-slip wall, the turbulent kinetic energy is set to zero on the wall, i.e. $\hat{k}_{wall} = 0$. Furthermore, following Wilcox [138] and Menter [88], the values of $\hat{\omega}$ near the wall are computed from

$$\hat{\omega}_{wall} = 60 \frac{\mu_k}{\rho_k \beta_{1,k} (d_k)^2}, \quad (4.46)$$

where k denotes the index of the cell, d is the distance from the wall to the centroid of the inner cell, μ is the molecular viscosity, and β_1 is a constant in SST formulation (see e.g. [90]).

In this thesis, adiabatic solid walls are considered, i.e. the normal component of the heat flux vector is taken equal to zero at the wall. This implies that the component of the gradient of the internal energy normal to the wall must also be equal to zero. The values of the remainder of the variables on the solid boundaries depend on the flow field solution and need to be extrapolated to the halo cells. Note that, for the extrapolation of the scalar variables such as density and pressure, it is allowed to take the gradient normal to the wall equal to zero, because the resolution of the computational grid in the wall normal direction is rather fine (to capture the boundary layer). Hence, given the

internal cell values $\mathbf{U}_{k_n} = [\rho, \mathbf{u}^T, \rho E]^T_{k_n}$, and the variables $(\hat{U}_{k_n})_{S-A} = \hat{\nu}$ when using the S-A turbulence model and $(\hat{U}_{k_n})_{SST} = [\rho \hat{k}, \rho \hat{\omega}]^T$ when using the SST turbulence model, the halo cell values are the following

$$\mathbf{U}_{h_n} = \begin{bmatrix} \rho \\ -\mathbf{u} \\ \rho E - 2(\rho \hat{k})_{SST} \end{bmatrix}_{k_n}, \quad (4.47)$$

$$(\hat{U}_{h_n})_{S-A} = -(\hat{U}_{k_n})_{S-A} \quad \text{or} \quad (\hat{U}_{h_n})_{SST} = \begin{bmatrix} -(\hat{U}_{1,k_n})_{SST} \\ 2\rho \hat{\omega}_{wall} - (\hat{U}_{2,k_n})_{SST} \end{bmatrix}, \quad (4.48)$$

where, the last component of $\mathbf{U}_{h_n}$ is an extrapolation of the total energy using the values of the turbulent kinetic energy $\hat{k}_{k_n} \equiv \frac{1}{2}(\mathbf{u}_t \cdot \mathbf{u}_t)_{k_n}$ (in the case of the SST turbulent model), with $\mathbf{u}_t$ denoting the turbulent velocity fluctuations.

4.3.5 MUSCL schemes

The reconstruction of the variables in the MUSCL-type schemes can be obtained using the following formulation

$$\mathbf{U}_{kl}^- = \bar{\mathbf{U}}_k + \Phi_{kl}^- ((\nabla \mathbf{U})_k \cdot (\mathbf{x}_{kl} - \mathbf{x}_k)), \quad (4.49)$$

$$\mathbf{U}_{kl}^+ = \bar{\mathbf{U}}_l + \Phi_{kl}^+ ((\nabla \mathbf{U})_l \cdot (\mathbf{x}_{kl} - \mathbf{x}_l)). \quad (4.50)$$

Here, the $-$ and $+$ superscripts denote the left and right state of a cell face, respectively. Furthermore, $\mathbf{U}_{kl}^\pm$ are the reconstructed variables at the left and right states of face kl , $\nabla \mathbf{U}$ is the gradient of the variables in the centroid of a cell, and $\mathbf{x}$ denotes the coordinates of a point. Moreover, Φ is vector of the limiter functions. The MUSCL schemes use the limiter functions in order to prevent spurious oscillations in the flow solution, especially near discontinuities and sharp gradients. The limiter functions that are used in this thesis satisfy the Total Variation Diminishing (TVD) property (see Harten [44]). The TVD schemes aim at preventing the generation of new extrema in the flow solution and are thus monotonicity-preserving.

There is a variety of choices for the limiter function Φ that can be found in the literature. The most trivial case is for $\Phi_j = 1$, which results in a linear scheme that is second order accurate for smooth solutions. However, linear schemes are not TVD and thus result in non-physical reconstructed values in regions where the solution is not smooth. In order to guarantee a monotonic solution, the MinMod (see e.g. [77]) and Venkatakrishnan limiters [131] are employed in this thesis. The MinMod limiter is used for the structured grids. For the unstructured grids the Venkatakrishnan limiter is employed. These limiters are described below. The formulation for the limiters is presented for the left state of the cell face. Applying the limiter function to the right state of the face is similar and is therefore not included here.

MinMod limiter

The MinMod limiter is known as one of the most stable TVD limiters. When this limiter is used the numerical dissipation is to some extent higher than that for the other TVD limiters, but due to the complexities of cavitating flows a highly stable limiter is found to be necessary. Using a grid stencil $I := [k - 1, k, k + 1]$ which includes the current cell k and its neighboring cells, the ratio of the successive gradients $\mathbf{r}_k$ is defined as follows

$$\mathbf{r}_k = \frac{\bar{\mathbf{U}}_{k+1} - \bar{\mathbf{U}}_k}{\bar{\mathbf{U}}_k - \bar{\mathbf{U}}_{k-1}}. \quad (4.51)$$

Using $\mathbf{r}_k$, the MinMod limiter for the reconstructed variables on the left state of the cell face $k + 1/2$, which is shared between the cells k and $k + 1$, is defined as follows

$$\Phi_{k+1/2}^-(\mathbf{r}_k) = \begin{cases} \min(\mathbf{r}_k, 1) & \text{if } \mathbf{r}_k > 0 \\ 0 & \text{if } \mathbf{r}_k \leq 0 \end{cases}. \quad (4.52)$$

In this thesis the MinMod limiter is used for the test cases involving structured grids.

Venkatakrishnan limiter

Define the unlimited reconstructed values on the face $k + 1/2$ as

$$\hat{\bar{\mathbf{U}}}_{k+1/2}^- \equiv \mathbf{U}_{k+1/2}^-(\Phi_{k+1/2,j} = 1), \quad (4.53)$$

let Δ_- be equal to

$$\Delta_- = \hat{\bar{\mathbf{U}}}_{k+1/2}^- - \bar{\mathbf{U}}_k, \quad (4.54)$$

and let Δ_+ be defined by

$$\Delta_+ = \begin{cases} \bar{\mathbf{U}}_k^{\max} - \bar{\mathbf{U}}_k & \text{if } \Delta_- > 0 \\ \bar{\mathbf{U}}_k^{\min} - \bar{\mathbf{U}}_k & \text{if } \Delta_- < 0 \end{cases}, \quad (4.55)$$

where $\bar{\mathbf{U}}_k^{\max}$ and $\bar{\mathbf{U}}_k^{\min}$ are the maximum and minimum values of the cell centered solutions within the employed stencil of the grid, respectively. Then the Venkatakrishnan limiter is given by

$$\Phi_{k+1/2}^- = \frac{\Delta_+^2 + \epsilon^2 + 2\Delta_- \Delta_+}{\Delta_+^2 + 2\Delta_-^2 + \Delta_- \Delta_+ + \epsilon^2}, \quad (4.56)$$

where $\epsilon^2 = (K\Delta x)^3$. Here, Δx is the grid size, and K is a coefficient which is simulation dependent (see Venkatakrishnan [131]). In the present thesis, the Venkatakrishnan limiter is used for numerical simulation of the viscous flow, in which, for both steady and unsteady flow simulations, a value $K = 0$ is adopted.

4.3.6 Time integration

In order to guarantee the monotonicity of the flow solution, the employed time integration schemes in this thesis satisfy the TVD property. The explicit multistage Runge-Kutta

scheme of Jameson *et al.* [57], explicit third order accurate three-stage TVD Runge-Kutta method (Shu [120]), and dual time integration methods are considered.

Explicit Runge-Kutta schemes

Assuming $\mathbf{U}_k^n$ as the vector of variables at time step n , the multi-stage Runge-Kutta scheme [57], $\mathbf{U}_k^{n+1}$ is obtained from the following formulation

$$\mathbf{U}_k^1 = \mathbf{U}_k^n, \quad (4.57)$$

$$\mathbf{U}_k^{(m+1)} = \mathbf{U}_k^1 + \alpha_{m+1} \Delta t \mathfrak{R}_k \left(\mathbf{U}_k^{(m)} \right), \quad m = \{1, \dots, \mathcal{M}\} \quad (4.58)$$

$$\mathbf{U}_k^{n+1} = \mathbf{U}_k^{(\mathcal{M}+1)}, \quad (4.59)$$

where α_{m+1} is the Runge-Kutta coefficient. For consistency, we require $\alpha_{\mathcal{M}+1} = 1$, and the scheme is second order accurate in time if $\alpha_m = 1/2$ (see e.g. Blazek [9]).

Additionally, a third order accurate three-stage TVD Runge-Kutta scheme is used which is given by

$$\mathbf{U}_k^{(1)} = \mathbf{U}_k^n + \Delta t \mathfrak{R}_k (\mathbf{U}_k^n), \quad (4.60)$$

$$\mathbf{U}_k^{(2)} = \frac{3}{4} \mathbf{U}_k^n + \frac{1}{4} \mathbf{U}_k^{(1)} + \frac{1}{4} \Delta t \mathfrak{R}_k \left(\mathbf{U}_k^{(1)} \right), \quad (4.61)$$

$$\mathbf{U}_k^{(n+1)} = \frac{1}{3} \mathbf{U}_k^n + \frac{2}{3} \mathbf{U}_k^{(2)} + \frac{2}{3} \Delta t \mathfrak{R}_k \left(\mathbf{U}_k^{(2)} \right). \quad (4.62)$$

When using explicit schemes for cavitating flows, the time step Δt must be taken rather small such that the details of the propagation of pressure waves are resolved. Furthermore, at each time step the CFL condition is checked using the following definition

$$\mathcal{C} = \frac{\Delta t_k}{\min \left(\frac{|V_k|}{\lambda_k^c}, \frac{|V_k|}{\lambda_k^v} \right)}, \quad (4.63)$$

where, $\mathcal{C}$ is the CFL number, $|V_k|$ is the volume of the cell k , and λ_k^c and λ_k^v are the convective and viscous spectral radii in the cell k which are computed as follows

$$\lambda_k^c = \sum_{l=1}^{N_{S,k}} (|\mathbf{u}_{kl} \cdot \mathbf{n}_{kl}| + c_{kl}) |\mathbf{S}_{kl}|, \quad (4.64)$$

$$\lambda_k^v = \sum_{l=1}^{N_{S,k}} \frac{C}{\rho_{kl}} \left(\frac{4}{3} (\mu_{kl} + \hat{\mu}_{kl}) + \gamma_{kl} \left(\frac{\mu_{kl}}{Pr} + \frac{\hat{\mu}_{kl}}{\hat{Pr}} \right) \right) \frac{\Delta \mathbf{x}_{kl} \cdot \mathbf{S}_{kl}}{|\Delta \mathbf{x}_{kl}|^2}, \quad (4.65)$$

where $\Delta \mathbf{x}_{kl}$ is the vector joining the cell centers k to the neighboring cell center l . These expressions are written by using the definition for the mean value of a variable φ on the cell face kl with $\varphi_{kl} = (\varphi_k + \varphi_l)/2$. Furthermore, u_{kl} and c_{kl} are the velocity and speed of sound, respectively, μ_{kl} and $\hat{\mu}_{kl}$ are the laminar and eddy viscosity (in a turbulent calculation), respectively, and ρ_{kl} and γ_{kl} are the density and specific heat ratio, respectively. Moreover, C is a constant, which, following Mavriplis & Jameson [86], is

taken as $C = 4$. The coefficient $4/3$ comes from the eigenvalue analysis for computing the spectral radius.

Dual time stepping

In the dual time-stepping strategy [55], [56], an implicit time integration scheme is employed, which in our case is the second order accurate BDF scheme:

$$\left(\frac{d\mathbf{U}}{dt}\right)^{n+1} = \frac{1}{2\Delta t} (3\mathbf{U}^{n+1} - 4\mathbf{U}^n + \mathbf{U}^{n-1}). \quad (4.66)$$

The solution for each time level $n + 1$ is considered as a steady flow problem, for which, all of the well known convergence acceleration techniques can be used. For the dual time stepping approach, an additional time derivative is added to equation (4.21) in order to account for the evolution of the pseudo time steps. The dual time stepping formulation can be written as follows

$$\frac{\partial \mathbf{U}_k}{\partial \tau} + \mathfrak{R}^*(\mathbf{U}_k) = 0, \quad (4.67)$$

where, τ denotes the pseudo time and

$$\mathfrak{R}^*(\mathbf{U}_k) = \frac{3\mathbf{U}_k - 4\mathbf{U}_k^n + \mathbf{U}_k^{n-1}}{2\Delta t} - \mathfrak{R}(\mathbf{U}_k), \quad (4.68)$$

is a second-order accurate implicit time discretization of equation (4.21). Using a backward Euler scheme for the discretization of equation (4.67) and after linearization of $\mathfrak{R}(\mathbf{U}_k)$, the solution at each pseudo time step $m + 1$ can be found from the following formulation

$$\left(\frac{\underline{I}}{\Delta \tau} + \frac{3\underline{I}}{2\Delta \tau} + \underline{A}(\mathbf{U}_k)\right) \Delta \mathbf{U}_k = -\mathfrak{R}^*(\mathbf{U}_k^m), \quad (4.69)$$

where, $\Delta \mathbf{U}_k = \mathbf{U}_k^{m+1} - \mathbf{U}_k^m$, $\Delta \tau$ is the pseudo time step, $\underline{I}$ is the identity matrix, and $\underline{A}(\mathbf{U}_k) = \left(\frac{\partial \mathfrak{R}(\mathbf{U})}{\partial \mathbf{U}}\right)_k$ is the Jacobian of $\mathfrak{R}(\mathbf{U})$. In this thesis, the dual time stepping approach is not used in its fully implicit form presented in equation (4.69). Instead, an explicit dual time stepping approach is pursued, which is obtained by omitting the Jacobian $\underline{A}(\mathbf{U}_k)$ in equation (4.69). The resulting explicit dual time stepping scheme is relatively simple and computationally less expensive than the fully implicit scheme. However, the scheme is only conditionally stable and hence the pseudo time step $\Delta \tau$ must obey the CFL criterion, see equation (4.63). The explicit dual stepping approach can also be obtained by using the Runge-Kutta scheme. When using a multi-stage Runge-Kutta scheme, the discretized form of equation (4.67) is given by

$$\frac{\mathbf{U}_k^{m+1} - \mathbf{U}_k^1}{\Delta \tau} + \alpha_{m+1} \mathfrak{R}^*(\mathbf{U}_k^{m+1}) = 0, \quad m = \{1, \dots, \mathcal{M}\}, \quad (4.70)$$

where α_{m+1} is the Runge-Kutta coefficient. The residual in equation (4.70) is then linearized, and, following the explicit dual time integration approach described before, the Jacobian term is set to zero. Pursuing a low-storage approach, which is obtained by setting $\mathbf{U}_k^1 = \mathbf{U}_k^m$, equation (4.70) can thus be rewritten as follows

$$\left(\frac{1 + \frac{3\Delta \tau}{2\Delta t} \alpha_{m+1}}{\alpha_{m+1} \Delta \tau}\right) \Delta \mathbf{U}_k = -\mathfrak{R}^*(\mathbf{U}_k^m). \quad (4.71)$$

4.4 WENO scheme

Weighted Essentially Non-Oscillatory (WENO) schemes (Liu *et al.* [82], Jiang & Shu [58]) perform polynomial reconstruction of variables in an adaptive stencil manner such that using the local smoothness indicators of the solution, the smoothest solution is automatically chosen in order to achieve a high-order accurate solution with no (or rather small) oscillations near the discontinuities. In the following the finite volume WENO reconstruction scheme is described (based on Shu [121]).

4.4.1 One-dimensional reconstruction

Reconstruction from cell average values

A 1D computational grid with $k = \{1, 2, \dots, N\}$ cells is defined. Each cell I_k is defined as $x_{k-1/2} \leq x \leq x_{k+1/2}$, with $\Delta x_k = x_{k+1/2} - x_{k-1/2}$. A scalar solution $q(x)$ is considered. Given the cell averages of $q(x)$ in cell I_k :

$$\bar{q}_k \equiv \frac{1}{\Delta x_k} \int_{x_{k-1/2}}^{x_{k+1/2}} q(\varphi) d\varphi, \quad k = 1, \dots, N, \quad (4.72)$$

a polynomial $p_k(x)$ of degree at most $(m-1)$ is sought, such that the polynomial is a m -th order accurate approximation of function $q(x)$ inside cell I_k , i.e.,

$$p_k(x) = q(x) + O(\Delta x^m), \quad x \in I_k, k = 1, \dots, N. \quad (4.73)$$

In particular, this gives a m -th order accurate approximation to the function $q(x)$ at the cell faces

$$q_{k+1/2}^- = p_k(x_{k+1/2}), \quad q_{k-1/2}^+ = p_k(x_{k-1/2}), \quad k = 1, \dots, N. \quad (4.74)$$

Given the location I_k and the order of accuracy m , a stencil

$$S(k) := \{I_{k-r}, \dots, I_{k+s}\} \quad (4.75)$$

based on r cells to the left, s cells to the right of I_k , with $r + s + 1 = m$ ($r, s \geq 0$) is considered. It can be shown that there is a unique polynomial $p_k(x)$ of degree at most $m-1 = r+s$, with the cell average in each cell of $S(k)$ given by

$$\frac{1}{\Delta x_j} \int_{x_{j-1/2}}^{x_{j+1/2}} p(\varphi) d\varphi = \bar{q}_j, \quad j = k-r, \dots, k+s, \quad (4.76)$$

which is similar to the cell averages of $q(x)$.

Let us define the location of a point inside a cell k by x_{k+k_c} , such that

$$-1/2 \leq \frac{x_{k+k_c} - x_k}{\Delta x_k} \leq 1/2. \quad (4.77)$$

Since the mapping from the cell averages $\bar{q}_k$ in the stencil $S(k)$ to the values of $q_{k+k_c}(x_{k+k_c})$ inside cell k and in particular the mapping to the face values $q_{k+1/2}^-$ and $q_{k-1/2}^+$ in equation (4.74) is linear, there exist constants c_{rj} , such that

$$q_{k+k_c}^{(r)} = \sum_{j=0}^{m-1} c_{rj} \bar{q}_{k-r+j}, \quad r = 0, \dots, m-1. \quad (4.78)$$

Note that c_{rj} is grid-dependent but it is not dependent on the function q itself. The expression for c_{rj} is derived using the Lagrange polynomial approximations (see Shu [121]). For a location x_{k+k_c} inside cell I_k in the stencil $S(k)$ (equation (4.75)) the expression for c_{rj} is given by

$$c_{rj} = \left(\sum_{b=j+1}^m \frac{\sum_{l \neq b}^m \prod_{i \neq b, l}^m (x_{k+k_c} - x_{k-r+i-1/2})}{\prod_{l \neq b}^m (x_{k-r+b-1/2} - x_{k-r+l-1/2})} \right) \Delta x_{k-r+j}. \quad (4.79)$$

For the reconstruction of the variables on the cell faces, i.e. $q_{k \pm 1/2}^\mp$, the c_{rj} coefficient is obtained by setting $x_{k+k_c} \equiv x_{k \pm 1/2}$ in equation (4.79). Note that, when the stencil $S(k)$ in equation (4.75) is utilized to reconstruct the variables on both the left and right states of a face $k + 1/2$, i.e. $q_{k+1/2}^\mp$, an additional left shift with $r = -1$ is also considered in equation (4.78), such that we have $-1 \leq r \leq m-1$.

In the current thesis, structured grids are considered for numerical simulations using the WENO scheme. When a uniform structured grid is used, given the order of accuracy of the approximations m , the c_{rj} coefficients in equation (4.79) on the cell faces are simplified to constant values (the values of these constants can be found in Shu [121]). In the current thesis non-uniform structured grids are also considered. For the non-uniform grids, the coefficients c_{rj} are grid-dependent. For example, the coefficients c_{rj} for a polynomial approximation with $m = 2$ can be found in Appendix F. Moreover, since the values of the c_{rj} coefficients are grid-dependent (and not solution-dependent), for a non-deforming grid, in order to reduce computational costs the c_{rj} coefficients can be computed and stored at the start of the computations.

WENO approximation

Within the stencil $S(k)$ in equation (4.75), given $0 \leq r \leq m-1$, there are m different candidate sub-stencils defined by

$$S_r(k) := \{x_{k-r}, \dots, x_{k-r+m-1}\}, \quad (4.80)$$

that can be used for a m -th order accurate polynomial approximation of $q(x_{k+k_c})$ inside cell k . The WENO scheme uses a convex combination of the m polynomials on $S(k)$ in order to obtain a non-oscillatory $(2m-1)$ th-order accurate approximation of $q(x_{k+k_c})$:

$$q_{k+k_c} = \sum_{r=0}^{m-1} w_r p_{k+k_c}^{(r)}, \quad (4.81)$$

where w_r are nonlinear weights. For consistency and stability, it is required that $w_r \geq 0$ and $\sum_{r=0}^{m-1} w_r = 1$. If the function $q(x)$ is smooth in all the candidate substencils $S_r(k)$ in equation (4.80), then there are constants d_r such that

$$q_{k+k_c} = \sum_{r=0}^{m-1} d_r p_{k+k_c}^{(r)} + O(\Delta x^{2m-1}), \quad (4.82)$$

where, due to consistency, we have $d_r \geq 0$ and $\sum_{r=0}^{m-1} d_r = 1$. In Appendix F the d_r weights (also called ideal weights) for a third-order accurate WENO scheme (with $m = 2$) are presented.

In case of a smooth solution it is desired that

$$w_r = d_r + O(\Delta x)^{m-1}. \quad (4.83)$$

If this is satisfied, then the approximated q_{k+k_c} variables in equation (4.81) are $(2m-1)$ -th order accurate (because $O(w_r p_{k+k_c}^{(r)}) \equiv O(\Delta x)^{m-1} O(\Delta x)^m = O(\Delta x)^{2m-1}$), such that

$$q_{k+k_c} = \sum_{r=0}^{m-1} w_r p_{k+k_c}^{(r)} = q(x_{k+k_c}) + O(\Delta x^{2m-1}). \quad (4.84)$$

When the function $q(x)$ has a discontinuity in one or more of the substencils $S_r(k)$ in equation (4.80), the WENO scheme chooses the corresponding weight (s) w_r to be essentially zero, such that the reconstruction is performed using the smoothest stencil. The nonlinear weights w_r can be defined as

$$w_r = \frac{\alpha_r}{\sum_{s=0}^{m-1} \alpha_s}, \quad \alpha_r = \frac{d_r}{(\epsilon + \beta_r)^2}. \quad (4.85)$$

Here ϵ is a small parameter that prevents division by zero. This parameter is set to values within a range of $\epsilon \approx 10^{-5} - 10^{-7}$ (Jiang & Shu [58]). β_r is the smoothness indicator of the stencil $S_r(k)$. There are different ways to determine the smoothness indicators (see e.g. Shu [121] and Jiang & Shu [58]). In the current thesis, we use the measure taken from [58], which uses the sum of the squares of the scaled L_2 norms for the derivatives of the interpolation polynomial inside the cell I_k :

$$\beta_r = \sum_{l=1}^{m-1} \int_{x_{k-1/2}}^{x_{k+1/2}} (\Delta x)^{2l-1} \left(\frac{d^l p^{(r)}(x)}{dx^l} \right)^2 dx. \quad (4.86)$$

In Appendix F, the expressions for β_r for a third-order accurate WENO scheme (with $m = 2$) are presented.

WENO, boundary conditions

For periodic boundary conditions there are no specific requirements, only as many halo cells as needed are specified and a periodicity condition is used. For symmetry and solid wall boundary conditions, the required number of the halo cells is specified and the halo

cell values are specified using the procedures described in section 4.3.4. For the inflow and outflow boundaries only the farfield boundary condition is used in this thesis, which can be specified using the procedure described in section 4.3.4. However, when following the approach in section 4.3.4, one needs to specify more than one layer of halo cells, which is not a very efficient approach. To avoid this, one can specify only the first layer of the halo cells, and set the values of the additional layers to very large values with very large variations [121]. For example, one can set $q_{-k} = (10k)^{10}$ if x_{-k} , with $k = 2, 3, \dots$ for additional halo cells (and $k = 1$ for the first halo cell which is assigned to the farfield values). Using this approach, the WENO scheme automatically chooses only the smoothest stencil on the farfield boundaries, thus the additional halo cells with non-smooth values are avoided, and at the same time the accuracy of the scheme is preserved. This approach may also be applied to the symmetry and solid wall boundary conditions as well, such that only the first layer of the halo cells needs to be specified. However, it must be ascertained that the accuracy of the scheme is not decreased at these boundaries.

4.4.2 Multidimensional reconstruction WENO

An extension of the 1D finite volume WENO reconstruction to 2D/3D space is presented. When using a midpoint integration rule for computing the numerical fluxes over the cell faces, the reconstruction of the variables can be performed in each dimension separately (each one similar to a 1D reconstruction). However, this approach does not retain the high-order accuracy of the WENO scheme in the multidimensional case, because when using the midpoint rule the numerical scheme is at most second-order accurate in space. To retain the high-order accuracy of the WENO scheme in 2D/3D space, a multidimensional reconstruction needs to be performed (Shu [121,122], and Titarev & Toro [125]). In order to carry out a multidimensional reconstruction, two approaches can be pursued: genuine multidimensional reconstruction and dimension-by-dimension reconstruction (Titarev & Toro [125]). The genuine multidimensional reconstruction (Shi *et al.* [119]) considers all cells in the multidimensional stencil simultaneously in order to construct a reconstruction polynomial. In contrast, the dimension-by-dimension reconstruction (Casper & Atkins [15], and Shi *et al.* [119]) consists of a number of one-dimensional reconstruction sweeps. The dimension-by-dimension reconstruction is less complex and computationally less extensive than the genuine multidimensional reconstruction, in particular for 3D reconstruction [125]. In the current thesis, the dimension-by-dimension reconstruction approach is adopted, which is described below.

The Navier-stokes equations in semi-discretized form using a finite volume scheme have been presented in equation (4.21). For a multidimensional reconstruction, the inviscid residuals in equation (4.21) are obtained by computing the surface integrals over the cell faces in equation (4.1) using a Gauss quadrature rule. The residuals can then be written as

$$\mathcal{R}_k^c = -\frac{1}{|V_k|} \sum_{l=1}^{N_{S,k}} \sum_{i_g=0}^{N_g-1} \omega_{i_g} \mathbf{H} \left(\mathbf{U}_{kl,i_g}^-, \mathbf{U}_{kl,i_g}^+, n_{kl} \right) |\mathbf{S}_{kl}|, \quad (4.87)$$

where i_g denotes the index of the Gauss point on the cell face, N_g is the total number of the Gauss points, ω_{i_g} is the Gauss weight, and $\mathbf{U}_{kl,i_g}^-$ and $\mathbf{U}_{kl,i_g}^+$ are the vectors of the WENO reconstructed variables evaluated at the Gauss point locations at the left and right

Figure 4.2: Schematic of a 2D grid: stencils of face nodes needed for a third-order accurate WENO reconstruction of the variables at the Gauss points on two different cell faces, with cell centers (O), target cell (●), interface nodes (x), and Gauss quadrature points (■).

states of the cell face kl , respectively. In Figure 4.2 a schematic of a 2D Cartesian grid is presented, which shows the interface nodes required for a third-order accurate WENO reconstruction of the variables at the Gauss points on two different faces of a grid cell. In order to compute $\mathbf{U}_{kl,i_g}^\mp$ the WENO coefficients need to be computed at the Gauss quadrature points. In Appendix F, the expressions for computing the third-order accurate WENO (with $m = 2$) coefficients at an arbitrary point inside the cell are presented, which can also be used for computing the WENO coefficients at Gauss quadrature points.

For the third-order accurate multidimensional WENO reconstructions, a two-point Gauss quadrature (with $N_g = 2$) in 1D space defined by $x_{i_g} = \left\{ -\frac{\sqrt{3}}{6}, \frac{\sqrt{3}}{6} \right\}$, $x_{i_g} \in x_{ND}$ in cell I_k with $x_{ND} = \frac{x-x_k}{\Delta x_k}$ and $-\frac{1}{2} \leq x_{ND} \leq \frac{1}{2}$, and with $\omega_{i_g} = \left\{ \frac{1}{2}, \frac{1}{2} \right\}$, is utilized. Additionally, for fifth-order accurate multidimensional WENO reconstructions, a three-point Gauss quadrature (with $N_g = 3$) in 1D space defined by $x_{i_g} = \left\{ -\frac{\sqrt{15}}{10}, 0, \frac{\sqrt{15}}{10} \right\}$, $x_{i_g} \in x_{ND}$ and $\omega_{i_g} = \left\{ \frac{5}{18}, \frac{4}{9}, \frac{5}{18} \right\}$ is considered.

4.4.3 System of equations

The system of equations considered in the present thesis (section 2.4.1) are hyperbolic $n \times n$ systems. Let us consider the 1D Euler equations in conservation form:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = 0, \quad (4.88)$$

where, $\mathbf{q}$ and $\mathbf{f}$ are the vectors of the conservative variables and the fluxes, respectively:

$$\mathbf{q} = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u H \end{bmatrix}. \quad (4.89)$$

Equation (4.88) in quasi-linearized form can be written as follows:

$$\frac{\partial \mathbf{q}}{\partial t} + \underline{\underline{A}}(\mathbf{q}) \frac{\partial \mathbf{q}}{\partial x} = 0, \quad (4.90)$$

where,

$$\underline{A}(\mathbf{q}) \equiv \underline{J}(\mathbf{f}, \mathbf{q}) = \frac{\partial \mathbf{f}}{\partial \mathbf{q}}, \quad (4.91)$$

is the Jacobian matrix, which has n real eigenvalues

$$\lambda^1(\mathbf{q}) \leq \lambda^2(\mathbf{q}) \leq \dots \leq \lambda^n(\mathbf{q}), \quad (4.92)$$

with a corresponding set of independent (right) eigenvectors

$$\mathbf{r}^1(\mathbf{q}), \mathbf{r}^2(\mathbf{q}), \dots, \mathbf{r}^n(\mathbf{q}). \quad (4.93)$$

The matrix of the right eigenvectors $\underline{R}(\mathbf{q})$ whose columns are the eigenvectors in equation (4.93) is given by

$$\underline{R}(\mathbf{q}) = (\mathbf{r}^1(\mathbf{q}), \dots, \mathbf{r}^n(\mathbf{q})). \quad (4.94)$$

Furthermore, we have

$$\underline{R}^{-1}(\mathbf{q}) \underline{A}(\mathbf{q}) \underline{R}(\mathbf{q}) = \underline{\Lambda}(\mathbf{q}), \quad (4.95)$$

where $\underline{\Lambda}(\mathbf{q})$ is the diagonal eigenvalue matrix with the eigenvalues in equation (4.92) on its diagonal. Moreover, $\underline{R}^{-1}(\mathbf{q})$ is the matrix of the left eigenvectors, whose rows are the left eigenvectors denoted by $\mathbf{l}^1(\mathbf{q}), \dots, \mathbf{l}^n(\mathbf{q})$.

The WENO reconstruction of the variables can be performed either in a component-wise fashion or in a characteristic-wise fashion. The component-wise reconstruction of the variables for nonlinear system of equations can cause spurious oscillations in numerical simulations, which is due to the interaction of the discontinuities of different characteristic fields (see Harten *et al.* [45] and Qiu & Shu [100]). Therefore, the characteristic-wise reconstruction is preferred. In this approach the differences $\partial \mathbf{q}$ are transformed into locally transformed differences of characteristic variables $\partial \mathbf{w}$, given by

$$\partial \mathbf{w} = \underline{R}^{-1} \partial \mathbf{q}. \quad (4.96)$$

Using the characteristic transformation of the variables, the system of Euler equations in (4.90) is decomposed in a n -set system of scalar equations, which in 1D space can be written as

$$\frac{\partial \mathbf{w}}{\partial t} + \underline{\Lambda}(\mathbf{q}) \frac{\partial \mathbf{w}}{\partial x} = 0. \quad (4.97)$$

Let us consider the cell averages $\bar{\mathbf{q}}_k$, which are in the form of divided or undivided differences in the WENO scheme (see [122]), on a stencil $S(k)$ defined in equation (4.75). In the following, the procedure for characteristic-wise finite volume WENO reconstruction of $\mathbf{q}$ on the cell face at $x_{k+1/2}$ is described (based on [122]):

(a) Compute an average state $\bar{\mathbf{q}}_{k+1/2}$, which can be obtained using the following methods:

(i) A mean function given by $\bar{\mathbf{q}}_{k+1/2} = \frac{\bar{\mathbf{q}}_k + \bar{\mathbf{q}}_{k+1}}{2}$.

(ii) A mean function using primitive variable obtained from the cell averages given by $\bar{\mathbf{Q}}_k(\bar{\mathbf{q}}_k)$ and $\bar{\mathbf{Q}}_{k+1}(\bar{\mathbf{q}}_{k+1})$ to obtain $\bar{\mathbf{Q}}_{k+1/2}$, and then computing $\bar{\mathbf{q}}_{k+1/2}(\bar{\mathbf{Q}}_{k+1/2})$, which can sometimes be more stable than computing the mean value directly using $\bar{\mathbf{q}}$.

(iii) The Roe average formulation [104].

- (b) Compute the matrix of the left eigenvectors $\underline{R}^{-1}(\bar{\mathbf{q}}_{k+1/2})$.
- (c) Compute the transformed cell averages $\bar{\mathbf{w}}_k = \underline{R}^{-1}\bar{\mathbf{q}}_k$ for all k in the stencil $S(k)$.
- (d) Perform the scalar WENO reconstruction of each component of the characteristic variable $\bar{\mathbf{w}}_k$, to obtain the corresponding component of the reconstruction $\mathbf{w}_{k+1/2}^\pm$.
- (e) Transform back to physical space by using $\mathbf{q}_{k+1/2}^\pm = \underline{R}\mathbf{w}_{k+1/2}^\pm$.

In Appendix A.1 the eigenvalue and eigenvector matrices corresponding to the conservative variables are presented.

Using appropriate transformations, the conservative variables $\mathbf{q}$ can also be transformed to primitive variables or other desired variables. Equation (4.90) can be written in terms of primitive variables $\mathbf{Q}$ using the following transformation of the variables:

$$\partial\mathbf{Q} = \underline{P}_Q^{-1}\partial\mathbf{q}, \quad (4.98)$$

where, $\underline{P}_Q^{-1}$ is the inverse of the non-singular transformation matrix $\underline{P}_Q$ defined by

$$\underline{P}_Q \equiv \underline{J}(\mathbf{q}, \mathbf{Q}) = \frac{\partial\mathbf{q}}{\partial\mathbf{Q}}. \quad (4.99)$$

Then equation (4.90) can be rewritten as follows:

$$\frac{\partial\mathbf{Q}}{\partial t} + \underline{P}_Q^{-1}\underline{A}(\mathbf{Q})\frac{\partial\mathbf{Q}}{\partial x} = 0, \quad (4.100)$$

where $\underline{A}(\mathbf{Q})$ (equation (4.91)) is the flux Jacobian with respect to the primitive variables $\mathbf{Q}$. The variables in equation (4.100) can be decomposed to characteristic variables using a direct eigenvalue analysis. Alternatively, this can be done using the known information of $\underline{A}(\mathbf{q})$. Note that the term $\underline{P}_Q^{-1}\underline{A}(\mathbf{Q})$ in equation (4.100) can be written as:

$$\underline{P}_Q^{-1}\underline{A}(\mathbf{Q}) = \underline{P}_Q^{-1}\underline{A}(\mathbf{q})\underline{P}_Q = \underline{P}_Q^{-1}\underline{R}(\mathbf{q})\underline{\Lambda}(\mathbf{q})\underline{R}^{-1}(\mathbf{q})\underline{P}_Q. \quad (4.101)$$

Hence, using the matrices of the eigenvectors $\underline{R}(\mathbf{w}_Q) = \underline{P}_Q^{-1}\underline{R}(\mathbf{q})$ and $\underline{R}^{-1}(\mathbf{w}_Q) = \underline{R}^{-1}(\mathbf{q})\underline{P}_Q$ we can rewrite equation (4.100) in a characteristic form as follows:

$$\frac{\partial\mathbf{w}_Q}{\partial t} + \underline{\Lambda}(\mathbf{q})\frac{\partial\mathbf{w}_Q}{\partial x} = 0, \quad (4.102)$$

where,

$$\partial\mathbf{w}_Q = \underline{R}^{-1}(\mathbf{w}_Q)\partial\mathbf{Q}, \quad (4.103)$$

are the characteristic-wise primitive variables. Note that the eigenvalues $\underline{\Lambda}(\mathbf{q})$ in equations (4.102) and (4.97) are identical. In Appendix A.2 the eigenvalues and eigenvector matrices corresponding to different sets of primitive variables are presented. The presented characteristic-wise reconstruction approaches need to be extended to multidimensions. This is not straightforward, because in multidimensional case no unique direction of propagation of the characteristic variables exists. Hence, the coefficient matrices involved are not simultaneously diagonalizable [46]. Therefore, in the multidimensional case only the component-wise WENO reconstruction is considered.

4.5 Maximum principle

Although WENO schemes have proven their robustness in many applications, it is observed that the WENO-based simulations for cavitating flows fail near sharp gradients and discontinuities in flow field variables, which occur between different flow phases or near shock waves. This is due to the presence of rather small numerical oscillations near non-smooth solutions in the WENO reconstruction schemes. These (small) oscillations result in non-physical values of flow field variables such as density and/or internal energy. To avoid this issue, the numerical scheme must obey a maximum principle. In this section, first the maximum principle property is introduced. Then, the maximum principle-preserving WENO scheme proposed by Zhang & Shu [142] is presented. Finally, in section 4.5.2 a novel positivity-preserving (a family of maximum principle-preserving schemes) strategy for WENO is developed.

The following description of the maximum principle-preserving WENO scheme, is based on the work of Zhang & Shu [142]. A 1D scalar conservation law is considered as follows

$$\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} = 0, \quad q(x, 0) = q_0(x), \quad (4.104)$$

where $q_0(x)$ is assumed to be a bounded variation function, such that $a \leq q_0(x) \leq b$ with

$$a = \min_x q_0(x), \quad b = \max_x q_0(x) \quad (4.105)$$

The main difficulty in solving equation (4.104) is that the solution may contain sharp gradients and discontinuities even if the initial solution is smooth. Therefore, the physically relevant unique weak solution of the system, i.e. the solution that satisfies the entropy condition, must be considered. An important property of the solution that satisfies the entropy condition is that it satisfies a strict maximum principle (e.g. see Dafermos [22]) such that, given the bounded initial solution $q_0(x)$, we have $q(x, t) \in [a, b]$ for any x and t . Although WENO schemes are nonlinearly stable in numerical experiments, in general they do not satisfy a strict maximum principle [142]. It is not straightforward to obtain a uniformly high order accurate scheme satisfying a strict maximum principle in the sense that the numerical solution is never outside the range $[a, b]$.

TVD schemes satisfy a strict maximum principle. However, for the finite difference or finite volume TVD schemes solving equation (4.104), when the total variation is measured by that of the grid values, they necessarily degenerate to first order accuracy at smooth extrema (Cockburn *et al.* [18]). The TVD schemes are thus at most second order accurate in the L^1 norm for general smooth and non-monotone solutions. By measuring the total variation of the reconstruction polynomials, higher-order accurate (higher than second order accurate) TVD schemes can be developed (see e.g. Sanders [106], and Zhang & Shu [141]). However, it is not straightforward to generalize these schemes to multi-dimensional problems [142]. Moreover, WENO schemes do not strictly satisfy the TVD property. Therefore, WENO schemes do not strictly preserve the maximum principle, although they can reach high-order accuracy for smooth solutions. To get a genuinely high order accurate scheme satisfying the maximum principle, the maximum of the reconstruction polynomials must be measured. Based on such measurements, Zhang & Shu [142] developed a high order accurate maximum-principle-satisfying scheme for one-dimensional and multi-dimensional scalar conservation laws, which is described in the following.

To control the extremum of the reconstruction polynomials, the scaling limiter introduced by Liu & Osher [81] is used. This control is achieved by a linear scaling around the cell average. To demonstrate this, we consider a quadratic polynomial $p_k(x)$ approximating a function $q_k(x)$ with third order accuracy on an interval $I_k = [x_{k-1/2}, x_{k+1/2}]$. Let $\bar{q}_k^n$ denote the cell average of $q_k(x)$ at computational time t^n and $b_k = \max_{x \in I_k} (p_k(x))$, $a_k = \min_{x \in I_k} (p_k(x))$, define $\tilde{p}_k(x)$ as

$$\tilde{p}_k(x) = \theta (p_k(x) - \bar{q}_k^n) + \bar{q}_k^n, \quad \theta = \min \left\{ \left| \frac{b - \bar{q}_k^n}{b_k - \bar{q}_k^n} \right|, \left| \frac{a - \bar{q}_k^n}{a_k - \bar{q}_k^n} \right|, 1 \right\}, \quad (4.106)$$

where a and b are defined in equation (4.105). If $\bar{q}_k^n \in [a, b]$, then $\tilde{p}_k$ is still a third order accurate approximation with the same cell average, and $\tilde{p}_k(x) \in [a, b]$, for all $x \in I_k$ (this is proved in [81]). However, to construct a maximum principle-satisfying scheme, it is not straightforward to maintain the property $\bar{q}_k^n \in [a, b]$ during the time evolution, without destroying the accuracy. Following the idea by Perthame & Shu [96], Zhang & Shu [142] showed that under a suitable CFL condition, for a finite volume or similar scheme, the Strong Stability Preserving (SSP) (Gottlieb *et al.* [37]) or similar time discretization scheme will preserve the maximum principle property if the linear scaling equation (4.106) or a simplified version is used for the WENO reconstruction polynomials, therefore maintaining the uniform high order accuracy. The idea for the simplified limiter is to use the linear scaling limiter equation (4.106) by replacing the definition of a_k and b_k by:

$$a_k = \min_{x \in S_k} (p_k(x)), \quad b_k = \max_{x \in S_k} (p_k(x)), \quad (4.107)$$

with

$$S_k = \{x_{k-1/2} = \hat{x}_k^1, \hat{x}_k^2, \dots, \hat{x}_k^{N-1}, \hat{x}_k^N = x_{k+1/2}\}, \quad (4.108)$$

a finite set containing the Legendre Gauss-Lobatto quadrature points. Note that, since there is no need to evaluate the extrema of the polynomials in the simplified limiter, it can thus be implemented easily for polynomials of any degree.

4.5.1 Maximum principle satisfying finite volume WENO

A discretization of equation (4.104) using the finite volume WENO scheme in space and the forward Euler scheme in time, gives

$$\bar{q}_k^{n+1} = \bar{q}_k^n - \lambda_q \left[h_f(q_{k+1/2}^-, q_{k+1/2}^+) - h_f(q_{k-1/2}^-, q_{k-1/2}^+) \right], \quad (4.109)$$

where, n refers to the time step, and $\lambda_q = \frac{\Delta t}{\Delta x_k}$ is the ratio of the time step and the grid size. $\bar{q}_k^n$ is the cell averaged approximation of $q(x, t)$ in the cell $I_k = [x_{k-1/2}, x_{k+1/2}]$ at a time level n , and $q_{k\pm 1/2}^\mp$ are the high order WENO reconstructions of $\bar{q}_k^n$ on the cell faces. Furthermore, $h_f(q_L, q_R)$ is the numerical flux function, with q_L and q_R the reconstructed variables at the left and right states of the cell face. Following Zhang & Shu [142], let us consider a Lax-Friedrichs flux defined by

$$h_f(q_L, q_R) = \frac{1}{2} [f(q_L) + f(q_R) - \varrho_f(q_R - q_L)], \quad \varrho_f = \max |f'(q)|, \quad (4.110)$$

where, ϱ_f is the spectral radius of $f(q)$. This is a first order monotone flux scheme. For a monotone flux, a first order monotone scheme satisfies the strict maximum principle

(see the proof in [142]). However, when applying linear schemes with order of accuracy higher than one, for example the Lax-Wendroff scheme, the maximum principle is not satisfied any more (Godunov theorem [35]). Therefore, using nonlinear schemes such as the WENO scheme is essential to be able to achieve higher order accuracy near sharp gradients and near discontinuities in the flow field solution. However, as mentioned at the beginning of this section, WENO schemes do not strictly preserve the maximum principle property. Therefore, the maximum principle WENO scheme of Zhang & Shu [142] is used, which is described below.

Given the discretized equation (4.109), and assuming that $\bar{q}_k^n \in [a, b]$ for all k , the aim is to modify the nodal values $q_{k\pm 1/2}^\mp$ such that $\bar{q}_k^{n+1} \in [a, b]$. A sufficient condition for this can be obtained for a stencil based on Legendre Gauss-Lobatto quadrature points. The stencil S_k in equation (4.108), for a N -point ($N \geq 2$) Legendre Gauss-Lobatto quadrature rule, is considered which is exact for the integral of polynomials of degree up to $2N - 3$. Moreover, for the stencil S_k we define $\hat{q}_\alpha = p_k(\hat{x}_k^\alpha)$ for $\alpha = \{1, \dots, N\}$, and the quadrature weights $\hat{\omega}_\alpha$ for the interval $[-1/2, 1/2]$ such that $\sum_{\alpha=1}^N \hat{\omega}_\alpha = 1$. Choose N to be the smallest integer satisfying $2N - 3 \geq 2m - 1$ (for $(2m - 1)$ -th order accurate WENO scheme), then

$$\bar{q}_k^n = \frac{1}{\Delta x_k} \int_{I_k} p_k(x) dx = \sum_{\alpha=1}^N \hat{\omega}_\alpha \hat{q}_\alpha. \quad (4.111)$$

Let us consider the flux scheme in equation (4.110), on the stencil S_k in equation (4.108) on the interval I_k , and denote $\hat{q}_0 = q_{k-1/2}^-$ and $\hat{q}_{N+1} = q_{k+1/2}^+$. Note that we have

$$\begin{aligned} h_f(q_{k+1/2}^-, q_{k+1/2}^+) - h_f(q_{k-1/2}^-, q_{k-1/2}^+) &= h_f(\hat{q}_N, \hat{q}_{N+1}) - h_f(\hat{q}_0, \hat{q}_1) \\ &= \sum_{\alpha=1}^N [h_f(\hat{q}_\alpha, \hat{q}_{\alpha+1}) - h_f(\hat{q}_{\alpha-1}, \hat{q}_\alpha)]. \end{aligned} \quad (4.112)$$

Using equations (4.112) and (4.111), equation (4.109) can be rewritten as follows:

$$\begin{aligned} \bar{q}_j^{n+1} &= \sum_{\alpha=1}^N \hat{\omega}_\alpha \hat{q}_\alpha - \lambda_q [h_f(q_{k+1/2}^-, q_{k+1/2}^+) - h_f(q_{k-1/2}^-, q_{k-1/2}^+)] \\ &= \sum_{\alpha=1}^N \hat{\omega}_\alpha \left[\hat{q}_\alpha - \frac{\lambda_q}{\hat{\omega}_\alpha} [h_f(\hat{q}_\alpha, \hat{q}_{\alpha+1}) - h_f(\hat{q}_{\alpha-1}, \hat{q}_\alpha)] \right] = \sum_{\alpha=1}^N \hat{\omega}_\alpha H_{f,k}^\alpha, \end{aligned} \quad (4.113)$$

where

$$H_{f,k}^\alpha = \hat{q}_\alpha - \frac{\lambda_q}{\hat{\omega}_\alpha} [h_f(\hat{q}_\alpha, \hat{q}_{\alpha+1}) - h_f(\hat{q}_{\alpha-1}, \hat{q}_\alpha)], \quad \alpha = 1, \dots, N. \quad (4.114)$$

It is noticed that $H_{f,k}^\alpha$ in equation (4.114) has the same form as equation (4.109), with $\frac{\lambda_q}{\hat{\omega}_\alpha}$ in place of λ_q . Therefore, provided that $\hat{q}_\alpha$ ($\alpha = \{0, \dots, N+1\}$) and $\bar{q}_k^n$ are in the range $[a, b]$, then $H_{f,k}^\alpha \in [a, b]$ subject to a scaled CFL condition

$$\lambda_q \varrho \leq \tilde{C}, \quad \tilde{C} = \min(\hat{\omega}_\alpha) \mathcal{C}, \quad (4.115)$$

where $\tilde{\mathcal{C}}$ is the scaled CFL number ($\mathcal{C}$ is the original CFL number). If these conditions are satisfied then we have $\bar{q}_k^{n+1} \in [a, b]$ because $\bar{q}_k^{n+1}$ is a convex combination of $H_{f,k}^\alpha$, and the maximum principle is thus satisfied. Furthermore, given the order of accuracy of the approximations $2m - 1$ for a WENO scheme, the scaled CFL number $\tilde{\mathcal{C}}$ can be determined using the values of the weights ω_α for Legendre Gauss-Lobatto quadrature points in the stencil S_k on an interval $[-1/2, 1/2]$. In the following, CFL is given when using the third and fifth order accurate WENO schemes (with $m = 2$ and $m = 3$, respectively):

$$\begin{aligned} m = 2 \quad & \begin{cases} \text{quadrature points } \left\{ -\frac{1}{2}, 0, \frac{1}{2} \right\} \\ \text{quadrature weights } \left\{ \frac{1}{6}, \frac{2}{3}, \frac{1}{6} \right\} \end{cases} \quad \rightarrow \quad \tilde{\mathcal{C}} = \frac{1}{6}, \\ m = 3 \quad & \begin{cases} \text{quadrature points } \left\{ -\frac{1}{2}, -\frac{1}{\sqrt{20}}, \frac{1}{\sqrt{20}}, \frac{1}{2} \right\} \\ \text{quadrature weights } \left\{ \frac{1}{12}, \frac{5}{12}, \frac{5}{12}, \frac{1}{12} \right\} \end{cases} \quad \rightarrow \quad \tilde{\mathcal{C}} = \frac{1}{12}. \end{aligned} \quad (4.116)$$

Once the extrema on the Legendre Gauss-Lobatto quadrature points in S_k is determined, the scaling limiter in equation (4.106) is used to obtain the scaled reconstructed face values $\tilde{q}_{k-1/2}^+ = \tilde{p}_k(x_{k-1/2})$ and $\tilde{q}_{k+1/2}^- = \tilde{p}_k(x_{k+1/2})$. Then $\tilde{q}_{k\pm 1/2}^\mp$ is plugged into equation (4.109) to obtain a revised scheme given by:

$$\bar{q}_k^{n+1} = \bar{q}_k^n - \lambda_q \left[h_f(\bar{q}_{k+1/2}^-, \bar{q}_{k+1/2}^+) - h_f(\bar{q}_{k-1/2}^-, \bar{q}_{k-1/2}^+) \right], \quad (4.117)$$

which, subject to the CFL condition equation (4.115) satisfies the maximum principle.

It is noticed that the introduced maximum principle rule also holds for the multidimensional case, in particular for the multidimensional dimension-by-dimension reconstruction WENO scheme, as long as the maximum principle rule is applied to all multidimensional reconstructions. Furthermore, these results are derived using the global Lax-Friedrichs flux scheme, but they also hold for any other monotone flux scheme [142]. Finally, note that the framework for the maximum principle in this section is obtained for a scalar conservation law. This can be generalized to hyperbolic systems to preserve the maximum principle for certain physical quantities, such as e.g. density and pressure (see Zhang & Shu [143] and Zhang *et al.* [144]). In the present thesis, we do not follow these approaches for systems of equations. We adopt the maximum principle approach derived for the scalar quantities and apply it separately to the pair of independent thermodynamic variables (ρ, e) , i.e. density and internal energy.

Implementation for the third-order accurate WENO scheme

The implementation of the maximum principle satisfying scheme for a third-order accurate WENO scheme is presented (for a fifth-order scheme the reader is referred to [142]). Following the WENO reconstruction, the high-order reconstructed variables $q_{k-1/2}^+$ and $q_{k+1/2}^-$ on the faces of each cell I_k are available. To construct a high-order polynomial in order to apply the scaling limiter, the information from the cell averages and the reconstructed variables on the cell faces can be used. For the third order WENO scheme, the polynomial $p_k(x)$ is of degree two such that $p_k(x_{k-1/2}) = q_{k-1/2}^+$, $p_k(x_{k+1/2}) = q_{k+1/2}^-$ and the cell average of $p_k(x)$ over I_k is $\bar{q}_k^n$. Moreover, $p_k(x)$ should be a third

order accurate approximation to the exact solution on I_k . To obtain this, a Hermite type reconstruction of degree two is employed, such that, given $\bar{q}_k^n$ and $q_{k\pm 1/2}^\mp$, the polynomial $p_k(x)$ should satisfy:

$$\frac{1}{\Delta x_k} \int_{I_k} p_k(x) dx = \bar{q}_k^n, \quad p_k(x_{k-1/2}) = q_{k-1/2}^+, \quad p_k(x_{k+1/2}) = q_{k+1/2}^-. \quad (4.118)$$

if the reconstruction is written as

$$p_k(x) = a_2(x - x_k)^2 + a_1(x - x_k) + a_0, \quad (4.119)$$

then the coefficients can be determined explicitly as

$$a_0 = \frac{6\bar{q}_k^n - q_{k-1/2}^+ - q_{k+1/2}^-}{4}, \quad (4.120)$$

$$a_1 = \frac{q_{k+1/2}^- - q_{k-1/2}^+}{\Delta x_k}, \quad (4.121)$$

$$a_2 = \frac{3q_{k+1/2}^- - 6\bar{q}_k^n + 3q_{k-1/2}^+}{(\Delta x_k)^2}. \quad (4.122)$$

Assuming that the cell averages $\bar{q}_k^n$, and the WENO reconstruction of the variables on the cell faces ($q_{k\pm 1/2}^\mp$) for all k are available at time level n , the maximum principle procedure for a third order accurate WENO can be summarized as follows:

- Construct the Hermite polynomials $p_k(x)$.
- Evaluate the quadrature point values of $p_k(x)$ in S_k to determine a_k and b_k in equation (4.107).
- Apply the scaling limiter and compute $\tilde{p}_k(x)$ in (equation (4.106)).
- Compute the revised nodal values of $\tilde{q}_{k-1/2}^+ = \tilde{p}_k(x_{k-1/2})$ and $\tilde{q}_{k+1/2}^- = \tilde{p}_k(x_{k+1/2})$, then plug them into equation (4.117) with the CFL condition $\lambda \varrho \leq \frac{1}{6}$, to obtain the maximum principle satisfying third order accurate WENO approximations of equation (4.109) in the time level $n + 1$.

For the Runge-Kutta time discretization schemes, the scaling limiter must be applied at each stage/step of the Runge-Kutta scheme.

4.5.2 A novel positivity-preserving strategy for WENO in 1D

A novel positivity-preserving strategy for WENO scheme in 1D space is presented³. The 1D scalar conservation law in equation (4.104) is considered. For a scheme to be positivity-preserving, given an initial solution with $0 < q_0(x) < b$, the numerical solution $q(x, t)$ of equation (4.104) satisfies $q(x, t) > 0$.

³Part of the contents of this subsection is based on Ref. [66]

Scalar problem

Let us consider the discretized form of equation (4.104) presented in equation (4.109). It is assumed that for a function $q_k(x)$ with cell averages $\bar{q}_k^n$ in a cell $I_k = [x_{k-1/2}, x_{k+1/2}]$ at a time level n , $q_{k\pm 1/2}^\mp$ are the WENO reconstructed values of $q_k(x)$ on the cell faces. In order to preserve the positivity of $q(x)$ in space, the properties of the logarithmic transformations and inverse exponential transformations are employed. The basic idea is to perform the WENO reconstruction of the variables on a logarithmically transformed variable $\mathcal{Q}(x) = \ln(q(x))$ rather than $q(x)$ itself. The cell averages $\bar{q}_k^n$ are replaced by the transformed logarithmic values of the cell averages $\bar{\mathcal{Q}}_k^n = \ln(\bar{q}_k^n)$, such that:

$$\bar{\mathcal{Q}}_k^n = \frac{1}{\Delta x_k} \int_{I_k} p_k^n(x) dx, \quad (4.123)$$

where, $p_k^n(x)$ is the polynomial which approximates $\mathcal{Q}(x)$ in the cell I_k . The logarithmic cell averages $\bar{\mathcal{Q}}_k^n$ are then used for a WENO reconstruction of $\mathcal{Q}(x)$ on the cell faces, such that $\mathcal{Q}_{k\pm 1/2}^\mp = p_k^n(x_{k\pm 1/2}) \equiv \ln(\tilde{q}_{k\pm 1/2}^\mp)$ with $\tilde{q}_{k\pm 1/2}^\mp$ denoting the new reconstruction of $q_k(x)$ on the cell faces. The values of $\tilde{q}_{k\pm 1/2}^\mp$ are computed by performing an exponential transformation of $\mathcal{Q}_{k\pm 1/2}^\mp$, such that $\tilde{q}_{k\pm 1/2}^\mp = e^{\mathcal{Q}_{k\pm 1/2}^\mp}$. Therefore, $\tilde{q}_{k\pm 1/2}^\mp$ remains always positive. Then, $q_{k\pm 1/2}^\mp$ in equation (4.109) are replaced by $\tilde{q}_{k\pm 1/2}^\mp$ to compute $\bar{q}_k^{n+1}$. Moreover, the positivity property is also satisfied in time. The reason is that using the developed scheme, at a time level n , the positivity of $q(x)$ is preserved at any point in space, i.e. $q^n(x) > 0$ (and obviously $\bar{q}^n > 0$). Hence, when using a TVD time discretization scheme, the positivity of $\bar{q}^{n+1}$ must also be preserved, i.e. $\bar{q}^{n+1} > 0$.

Extension to system of equations

The developed positivity-preserving scheme for the scalar equations, is extended to a system of equations. The most trivial way is to apply the method in a component-wise manner, by reconstructing each component similar to the scalar case. However, it was found that the scheme works more effectively when the positivity-preserving reconstructions are performed using characteristic variables.

We consider the 1D Euler equations in quasi-linear form given in equation (4.90). Let us denote the desired positivity-preserving variables by

$$\mathbf{Q} = \begin{bmatrix} Q_1 \\ Q_2(u) \\ Q_3 \end{bmatrix}, \quad (4.124)$$

assuming that $Q_2(u)$ is a linear function of the velocity u , and it can get both negative and positive values. Then we transform $\mathbf{Q}$ to a semi-logarithmic form given by

$$\mathcal{Q} = \begin{bmatrix} \ln(Q_1) \\ Q_2 \\ \ln(Q_3) \end{bmatrix}. \quad (4.125)$$

Using a transformation of the conservative variables $\mathbf{q}$ to the new variables $\mathbf{Q}$, equation (4.90) can be transformed into primitive form given in equation (4.100). The new equation is obtained through replacing $\mathbf{Q}$ by $\mathbf{Q}$ in equation (4.100), which can be written as follows:

$$\frac{\partial \mathbf{Q}}{\partial t} + \underline{P}_{\mathbf{Q}}^{-1} \underline{A}(\mathbf{Q}) \frac{\partial \mathbf{Q}}{\partial x} = 0, \quad (4.126)$$

where $\underline{A}(\mathbf{Q})$ (equation (4.91)) is the flux Jacobian with respect to $\mathbf{Q}$, and $\underline{P}_{\mathbf{Q}} = \frac{\partial \mathbf{q}}{\partial \mathbf{Q}}$ is the transformation matrix.

In order to perform a characteristic-wise reconstruction of the variables $\mathbf{Q}$, a decoupling of the system of equation (4.126) is performed based on the transformed variables $\partial \mathbf{w}_{\mathbf{Q}} = \underline{R}^{-1}(\mathbf{Q}) \partial \mathbf{Q}$, with $\underline{R}(\mathbf{Q})$ the matrix of the right eigenvectors of $\underline{P}_{\mathbf{Q}}^{-1} \underline{A}(\mathbf{Q})$. The resulting scalar equations are:

$$\frac{\partial \mathbf{w}_{\mathbf{Q}}}{\partial t} + \underline{\Lambda}(\mathbf{q}) \frac{\partial \mathbf{w}_{\mathbf{Q}}}{\partial x} = 0, \quad (4.127)$$

where, $\underline{\Lambda}(\mathbf{q})$ are the diagonal matrix of the eigenvalues. In Appendix A.3 the matrices of eigenvalues and eigenvectors for logarithmically transformed variables are presented.

It is assumed that the space discretizations are performed using a high-order WENO scheme, and for a cell $I_k = [x_{k-1/2}, x_{k+1/2}]$ at time level n we have the cell averages $\bar{\mathbf{q}}_k^n$ with $\bar{\mathbf{q}}_k^n > 0$. The developed positivity-preserving approach for a system of equations to obtain the face values $\mathbf{q}_{k+1/2}^\pm$ on the face $k+1/2$ is summarized as follows:

- Using $\bar{\mathbf{q}}_k^n$ the desired positivity-preserving variables' cell averages $\bar{\mathbf{Q}}_k^n$, and the cell averaged semi-logarithmic variables $\bar{\mathbf{Q}}_k^n = [\ln(Q_{1,k}^n), Q_{2,k}^n, \ln(Q_{3,k}^n)]^T$ are computed.
- The matrix of eigenvectors $\underline{R}(\bar{\mathbf{Q}}_{k+1/2})$ is computed, where $\bar{\mathbf{Q}}_{k+1/2}$ is an average state (see the procedure in section 4.4.3).
- The cell-averaged characteristic-wise semi-logarithmic variables $\bar{\mathbf{w}}_{\mathbf{Q}_k}^n = \underline{R}^{-1}(\bar{\mathbf{Q}}_{k+1/2}) \bar{\mathbf{Q}}_k^n$ are computed.
- Each component of $\bar{\mathbf{w}}_{\mathbf{Q}_k}^n$ is reconstructed using the WENO scheme to obtain the face values $\mathbf{w}_{\mathbf{Q}_{k+1/2}}^n$.
- Through a reverse characteristic transformation, the semi-logarithmic face values $\mathbf{Q}_{k+1/2} = \underline{R}(\bar{\mathbf{Q}}_{k+1/2}) \mathbf{w}_{\mathbf{Q}_{k+1/2}}^n \equiv [\ln(Q_1))_{k+1/2}, (Q_2)_{k+1/2}, \ln(Q_3))_{k+1/2}]^T$ are computed.
- A reverse logarithmic mapping of the logarithmic components of $\mathbf{Q}_{k+1/2}$ is performed using exponential transformations to obtain the new face values $\mathbf{Q}_{k+1/2} = [e^{(\ln(Q_1))_{k+1/2}}, (Q_2)_{k+1/2}, e^{(\ln(Q_3))_{k+1/2}}]^T$.

Using this approach the desired components of the reconstructed variables $\mathbf{Q}_{k+1/2}$ remain always positive. Subsequently, the values of the conservative variables on the faces remain always positive, i.e. $\mathbf{q}_{k+1/2}(\mathbf{Q}_{k+1/2}) > 0$, and their cell-centered values after evolution in time (using a TVD time discretization scheme) also remain positive, i.e. $\bar{\mathbf{q}}^{n+1} > 0$.

4.6 Verification

The numerical framework described in the preceding sections is assessed. The accuracy of the different numerical schemes is checked using test cases with smooth solutions. Also, the performance of the schemes for problems with non-smooth solutions is assessed.

4.6.1 1D test case, accuracy study

The accuracy of the employed numerical schemes is assessed, based on the test case used in [82]. We consider the following scalar problem for a variable $q(x, t)$ with $x \in [-1, 1]$:

$$\frac{\partial q(x, t)}{\partial t} + \frac{\partial q(x, t)}{\partial x} = 0, \quad (4.128)$$

with the following conditions:

$$\begin{cases} q(x, 0) = \sin(\pi x) + 2 \\ \text{periodic boundary condition on } [-1, 1] \\ \text{integration time: } T = 0.18 \end{cases} \quad (4.129)$$

The numerical simulations are performed using the numerical framework described in preceding sections. The employed schemes include, the second-order accurate MUSCL scheme, third and fifth order accurate WENO schemes denoted by WENO3 and WENO5, respectively, and the developed positivity-preserving strategy for a the WENO3 scheme, denoted by log-WENO3. The time discretization is carried out using the three-stage third-order accurate TVD Runge-Kutta scheme (section 4.3.6).

In Table 4.1 the L^1 error norm and the order of the numerical schemes for different grid sizes is presented. Moreover, this data is visualized in Figure 4.3 to analyze the performance of the different schemes. These results are obtained using a CFL condition with $\mathcal{C} = 0.9$. However, note that for the WENO5 scheme (fifth order accurate) the usage of the third order accurate TVD Runge-Kutta scheme reduces the overall accuracy. In order to avoid this, at each grid refinement step, we would like to scale the CFL number such that the overall fifth order accuracy is recovered. Let us write equation (4.128) in discretized integral form as follows

$$\frac{d\bar{q}}{dt} + \frac{1}{\Delta x} (q_{k+1/2} - q_{k-1/2}) = 0, \quad (4.130)$$

for a cell k with $\bar{q}$ the cell centers and $q_{k\pm 1/2}$ are the cell face values. By carrying out a fifth order accurate spatial discretization and a third order accurate temporal discretization we have

$$(q_{k+1/2} - q_{k-1/2}) = \Delta x \mathfrak{R}_q(q, x) + O(\Delta x)^5, \quad (4.131)$$

$$\frac{d\bar{q}}{dt} = T_q(q, t) + O(\Delta t)^3, \quad (4.132)$$

where, $\mathfrak{R}_q$ and T_q are the numerically computed spatial residuals (defined in 4.23) and temporal derivative, respectively, and the second terms in the RHS of these equations are the truncation errors. For a starting grid level m (assuming a uniform grid) using

cell sizes Δx_m and a time step of Δt_m , we have the CFL condition with $C_m = \frac{\Delta t_m}{\Delta x_m}$. Then, keeping the CFL number constant, let us consider a refined grid size (grid level $m + 1$) and a smaller time step, with $\Delta x_{m+1} = \frac{1}{2}\Delta x_m$ and $\Delta t_{m+1} = \frac{1}{2}\Delta t_m$. The order of accuracy of the schemes can be computed by comparing the truncation errors of grid levels m and $m + 1$:

$$(r)_{\text{Tr},x} = \ln\left(\frac{(\Delta x_{m+1})^5}{(\Delta x_m)^5}\right) = \ln(2)^{-5}, \quad (4.133)$$

$$(r)_{\text{Tr},t} = \ln\left(\frac{(\Delta t_{m+1})^3}{(\Delta t_m)^3}\right) = \ln(2)^{-3}, \quad (4.134)$$

where, $(r)_{\text{Tr},x}$ and $(r)_{\text{Tr},t}$ are ratios of the spatial and temporal truncation errors, respectively, in logarithmic scale for the two cases. For level $m + 1$ (with refined grid), we would like to choose a time step $\Delta t_{m+1} = 2^a \Delta t_m < 2\Delta t_m$ such that the temporal order of accuracy is also fifth order, thus we would like to have

$$\ln\left(\frac{(2^a \Delta t_m)^3}{(\Delta t_m)^3}\right) = \ln 2^5, \quad (4.135)$$

which gives $a = -5/3$. Therefore, in order to preserve the accuracy of the WENO5 scheme for grid level $m + 1$ the scaled CFL number is computed from the following

$$(C)_{m+1}^{\text{WENO5}} = \frac{2^{-5/3} \Delta t_m}{1/2 \Delta x_m} = C_m \frac{2}{2^{5/3}} = 2^{-2/3} C_m. \quad (4.136)$$

The new value of CFL ensures that the temporal truncation error remains within the orders of the spatial truncation error. Note that, this is done only for the WENO5 scheme, because for the WENO3 and MUSCL schemes the spatial accuracy is within the order of accuracy of the temporal discretization, thus the expected accuracy is achieved.

The equation is integrated in time for a final time of $T = 0.18$. From Table 4.1, it is observed that the accuracy of the WENO3 and WENO5 schemes is as expected, i.e. third-and fifth-order accurate, respectively. However, the MUSCL scheme only approaches second order accuracy. This is because the MUSCL scheme uses limiter functions which are numerically dissipative, and thus decreasing the order of accuracy. Moreover, Figure 4.3 and Table 4.1 show that the developed positivity-preserving log-WENO3 scheme retains the third order accuracy up to a grid with $h = \frac{1}{320}$. However, in this case when the grid is refined further, the accuracy is decreased, such that it eventually becomes second order accurate. Furthermore, we have observed that the accuracy of a positivity-preserving log-WENO5 scheme for this problem (not included here) also becomes second order.

In order to improve the accuracy of the results, an alternative log-WENO-based reconstruction scheme has been developed for this test case. Given the cell averages $\bar{q}_k^n$, we perform the log-WENO reconstructions for a logarithmic variable $\ln(\bar{q}_k^n + C)$ rather than $\ln(\bar{q}_k^n)$ itself. In the new reconstruction, C is a constant which is chosen with large enough values in order to make sure that logarithmic values with relatively large gradients are avoided. The reason for this is because logarithmic values of q for this particular test case have relatively low values with relatively large gradients. These values are suspected to result in a WENO stencil with data that is not sufficiently smooth, and thus decreasing the order of accuracy. Here, we choose a value of $C = 10^3$ for the log-WENO3

Table 4.1: Accuracy study for test case defined in equation (4.128), for MUSCL, WENO3, WENO5, and the developed positivity-preserving Log-WENO3 schemes.

MUSCL			WENO3		log-WENO3		WENO5	
h	L^1 error	order	L^1 error	order	L^1 error	order	L^1 error	order
$\frac{1}{20}$	6.43E-03	-	5.86E-03	-	5.88E-03	-	4.64E-05	-
$\frac{1}{40}$	1.89E-03	1.77	1.39E-03	2.08	1.32E-03	2.15	1.48E-06	4.96
$\frac{1}{80}$	5.31E-04	1.83	2.81E-04	2.3	1.99E-04	2.73	4.61E-08	5.01
$\frac{1}{160}$	1.49E-04	1.83	2.41E-05	3.55	1.68E-05	3.57	1.43E-09	5.01
$\frac{1}{320}$	3.93E-05	1.92	1.47E-06	4.04	1.41E-06	3.58	4.43E-11	5.01
$\frac{1}{640}$	1.04E-05	1.92	8.7E-08	4.07	2.16E-07	2.71	1.41E-12	4.97

Figure 4.3: L^1 norm error, based on the test case in equation (4.128), for MUSCL, WENO3, WENO5, and the developed positivity-preserving log-WENO3 schemes, with N the number of the grid points, using $N = \{40, 80, 160, 320, 640, 1280\}$, and m denoting the slope.

and $C = 10^4$ for the log-WENO5, and we refer to the new reconstruction schemes as log+C-WENO3, and log+C-WENO5, respectively. After WENO reconstructions are obtained a reverse mapping is performed to obtain the final reconstructed values with $q_{k+1/2} = e^{\ln(q_{k+1/2}+C)} - C$.

The accuracy study for the log+C-WENO reconstruction approach is presented in Table 4.2 and Figure 4.3. From Table 4.2 it is observed that the log+C-WENO3 results are third-order accurate. We also observed that with further grid refinement (one level extra

Table 4.2: Accuracy study, for test case defined in equation (4.128), for the developed positivity-preserving Log+C-WENO3 and log+C-WENO5 schemes.

log+C-WENO3				log+C-WENO5		
h	L^1 error	order	Δt	L^1 error	order	Δt
$\frac{1}{20}$	1.58E-04	-	4.5E-02	4.3E-05	-	4.5E-02
$\frac{1}{40}$	1.98E-05	2.99	2.25E-02	1.37E-06	4.97	1.42E-02
$\frac{1}{80}$	2.48E-06	3.00	1.13E-02	4.27E-08	5.01	4.46E-03
$\frac{1}{160}$	3.19E-07	2.95	5.6E-03	1.32E-09	5.01	1.41E-03
$\frac{1}{320}$	3.93E-08	3.02	2.8E-03	1.48E-10	3.16	4.43E-04
$\frac{1}{640}$	4.88E-09	3.01	1.4E-03	3.67E-11	2.01	1.4E-04

refinement), the results remain third order accurate. Furthermore, the log+C-WENO5 results show that the initially achieved fifth accuracy is not maintained as the grid is refined. It is noticed that, as explained in the beginning of this section, at each grid level the CFL number is scaled in order to obtain fifth order accuracy in time. Therefore, the time discretization scheme should not play a role in the overall accuracy deficiency of the scheme. Moreover, note that the presented accuracy study only applies to the smooth parts of the numerical solution. For non-smooth solutions, the accuracy of the schemes near discontinuities reduces to first order accurate, which may also reduce the global accuracy of the solution to first order accurate. In contrast to the results for this test case, the log-WENO results (for both third-and fifth-order schemes) for different test cases which are presented in the next subsections (e.g. Sod's tube problem) are rather close to the results for the WENO scheme.

4.6.2 1D test case, positivity-preserving log-WENO scheme inside a single cell

A test case for the 1D Euler equations with a non-smooth solution is considered. The numerical simulations for this test case are performed using the third-order and fifth-order accurate WENO schemes denoted by WENO3 and WENO5, respectively, the developed positivity-preserving WENO scheme, denoted by log-WENO, and the Scaling Limiter (SL) maximum principle-satisfying WENO scheme [142] denoted by SL-WENO. At a time instance t^n of the numerical simulations, a grid cell k which contains a non-smooth solution is considered. Using the cell averages of cell k and its neighboring cells, the solution is reconstructed at all the points within cell k . This allows us to observe the performance of the numerical schemes, in particular to compare the performance of the log-WENO scheme with that of the SL-WENO scheme.

Figures 4.4a and 4.4b show plots of two non-smooth distributions of density ρ for WENO3 and WENO5 stencils, respectively, which are used for reconstruction of the values inside a target cell k .

Figure 4.4: Plots of density for 1D single-cell test case: (a), (b) cell averaged values of density (for two different cases) in WENO3 and WENO5 stencils, monotone cubic curves are used for visualization of the cell centered data (regardless of the accuracy); (c), (d) Distribution of the density in the stencil cells obtained using the monotone cubic scheme, and reconstructed values of the density using WENO, SL-WENO, and log-WENO schemes inside the target cell k ; (e), (f) Results for the density using the different WENO schemes inside cell k . The regions in which WENO coefficients are not defined are not shown.

Note that for the WENO scheme presented in section 4, the grid-dependent WENO coefficients are only defined in parts of the cell. Therefore, for the WENO results, the regions in which the WENO coefficients are not defined (in the middle part) are not shown. The plots show the entire computational domain, but only the data for the cell centers in the employed stencils are shown. In these figures, the circle symbols are the cell centers and the smoothened curves are obtained using the Monotone Piecewise Cubic Interpolation scheme (see e.g. Fritsch & Carlson [33]). Furthermore, Figures 4.4c and 4.4d show the cell centers in the employed stencils of WENO3 and WENO5 schemes, the reconstructed smoothened curves, and the WENO and positivity-preserving SL-WENO and log-WENO reconstructed values inside the target cell k . It is noticed that the smoothened monotone cubic interpolated curves use limiter functions (which were discussed in section 4.3) to preserve the monotonicity, thus reducing the accuracy of the interpolations. In particular their accuracy is not higher than first-order near the discontinuities. The monotone cubic interpolations are only used here for visualization of the cell-centered values (regardless of the accuracy of the interpolated data), and they are not used in the numerical simulations.

Furthermore, in Figures 4.4e, and 4.4f the WENO and positivity-preserving SL-WENO and log-WENO reconstructed values of the density inside the target cell k are presented. In these figures, the regions in which the WENO coefficients are not defined (in the middle region) are not shown. The plots are presented using a non-dimensional position $x_{ND} = \frac{x-x_0}{\Delta x}$ inside the cell, with x_0 denoting the cell-center location and Δx denoting the cell size. From Figure 4.4, it is observed that the original WENO scheme results in non-physical (negative) values for the density, in particular at the cell faces with $x_{ND} = \{-0.5, 0.5\}$. The SL-WENO and the log-WENO schemes successfully solve this problem, such that the reconstructed face values are positive.

It is noticed that the shape of the WENO curves in some parts is different from the smoothened monotone cubic curves. This is because the WENO scheme uses a combination of different stencil candidates of the cell centers using nonlinear weights. Each stencil candidate uses a part of the employed stencil's cells which is different from the other candidates and also different from the smoothened monotone cubic method (which is obtained using the data for all the cells in the employed stencil). Therefore, the interpolated values in each candidate stencil and subsequently in the final high-order accurate WENO interpolations (which are nonlinear combinations of the candidate stencil interpolations) are different from the low-order smoothened monotone cubic interpolations.

4.6.3 1D Sod's shock tube problem

In order to assess the employed numerical schemes for the system of equations with non-smooth solutions, Sod's classical shock tube problem [124] is solved. A tube with a dimensionless length of 1 is considered, which contains an ideal gas. Initially, a diaphragm in the middle of the tube divides the tube into two parts with different conditions. The conditions on the left and right sides of the diaphragm are $[\rho_L, u_L, p_L] = [1, 0, 1]$ and $[\rho_R, u_R, p_R] = [0.125, 0, 0.1]$, respectively. Here, ρ , p , and u are the dimensionless density, pressure, and velocity of the fluid, respectively. Moreover, the specific heat ratio of the gas is $\gamma = 1.4$. At a time $t = 0$ the diaphragm is removed instantly and the exact and the numerical solutions are computed until a final time of $T = 0.2$.

Figure 4.5: Numerical solutions for Sod's shock tube problem obtained analytically, and numerically using characteristic-wise (Cs) WENO3, WENO5, and MUSCL schemes, for the first four figures and the last two figures the number of grid cells is 100 and 600, respectively: (a) density; (b) magnified view of density; (c) velocity, with a magnified view shown in the middle part of the figure; (d) pressure, with a magnified view shown in the right side of the figure (e) density (refined grid); (f) magnified view of density plots (refined grid).

Figure 4.5 shows the plots for the exact solution and the numerical solutions obtained using the MUSCL scheme, with the limiter applied to the characteristic variables, and the third and fifth order accurate characteristic-wise (Cs) WENO reconstruction schemes (denoted by Cs-WENO3 and Cs-WENO5, respectively). Moreover, the time discretization is performed using the three-stage third-order accurate TVD Runge-Kutta scheme (section 4.3.6) with the CFL condition satisfying $\mathcal{C} = 0.4$ for all cases. Figures 4.5a, 4.5b, 4.5c, and 4.5d show the plots for density, velocity, and pressure, which are obtained using 100 grid cells. Furthermore, Figures 4.5e, and 4.5f show the plots of the density for a refined grid with 600 cells. From these figures, in particular from the magnified views of the density in Figures 4.5b and 4.5f, it is observed that near the discontinuities the results of the WENO5 scheme are sharper than those of the WENO3 and MUSCL schemes. Moreover, it is observed that the results of the WENO3 scheme are sharper than those of

Figure 4.6: Numerical simulations for Sod's shock tube problem for the density compared with analytical solution. Results for WENO and the developed positivity-preserved log-WENO schemes in characteristic (Cs) space, for the first two figures and the last two figures the number of grid cells are 100 and 600, respectively: (a) third-order accurate schemes; (b) fifth-order accurate schemes; (c) third-order accurate schemes (refined grid); (d) fifth-order accurate schemes (refined grid).

the MUSCL scheme.

In Figure 4.6 the plots of the density for Sod's shock tube problem computed using the characteristic-wise WENO3 and WENO5 schemes and characteristic-wise positivity-preserving log-WENO3 and log-WENO5 schemes are presented, and compared with the exact solution. Note that when using the WENO scheme for solving this problem, the positivity-preserving property is not needed. However, the positivity-preserving schemes are considered in order to assess their performance. Moreover, the results in Figures 4.6a, and 4.6b are obtained using 100 grid cells, and the results for a refined grid with 600 cells are shown in Figures 4.6c, and 4.6d. These figures show that, compared to the WENO scheme, near the discontinuities the log-WENO scheme solution has a good sharpness. Also, from a magnified view of the WENO5 plots shown in Figure 4.6b it is observed that the undershoots for the log-WENO5 scheme are smaller than for the WENO5 scheme in this part of the shock tube.

4.6.4 2D Burgers equation

The Burgers equation in 2D space is solved (see e.g. Shu [122] and Shabazi *et al.* [118]). Considering a rectangular domain with $x \in [-3, 3]$, $y \in [-3, 3]$ in dimensionless coordinates, the two-dimensional Burgers equation for a dimensionless scalar quantity $q(x, y, t)$ is given by

$$\frac{\partial q}{\partial t} + \frac{\partial (\frac{1}{2}q^2)}{\partial x} + \frac{\partial (\frac{1}{2}q^2)}{\partial y} = 0, \quad (4.137)$$

which, is solved using the following initial condition [122]:

$$q(x, y, 0) = 0.3 + 0.7 \sin\left(\frac{\pi}{3}(x + y)\right), \quad (4.138)$$

using periodic boundary conditions. The exact solution of this equation can be computed using the characteristic method (see e.g. LeVeque [75]). For the given initial conditions the solution is

$$q = 0.3 + 0.7 \sin\left(\frac{\pi}{3}((x - qt) + (y - qt))\right). \quad (4.139)$$

Equation (4.139) is an implicit expression for the solution $q(x, y, t)$. We solve equation (4.139) using Newton's linearization algorithm to obtain the final time $t = T$, for which the solution is still smooth.

When the characteristics intersect, shock waves are formed [75], i.e. the solution becomes discontinuous, and at time T_s equation (4.139) gives more than one solution at a position (x, y) , which physically is not possible. For Burgers equation, the initial formation time and location of the shock waves can be computed exactly (see e.g. [75] for 1D case). We follow the 1D approach to compute the initial time of formation and location of the shocks on a path s with

$$s : x = y, \quad (4.140)$$

such that equation (4.138) can be rewritten as

$$q_s(x, 0) = 0.3 + 0.7 \sin\left(\frac{2\pi}{3}x\right). \quad (4.141)$$

The initial shock time T_s on this path can be computed from the following [75]:

$$T_s = -\frac{1}{\min \frac{\partial}{\partial x} q_s(x, 0)}, \quad x \in [-3, 3], \quad (4.142)$$

Therefore, from above equation and using equation (4.141) we get the initial time of the shock as:

$$T_s = \frac{15}{7\pi}, \quad (4.143)$$

which correspond to positions $x_0 = \pm \frac{3}{2}$ at the time $t = 0$. Note that, using the characteristic method, for each position $x + y$ on a general path in equation (4.138) at a time t we have

$$x + y = (x + y)_0 + q(x, y, 0)t. \quad (4.144)$$

Therefore, given the path s in equation (4.140), at the initial time of the shock T_s the initial position of the shocks, i.e. x_s , can be computed from the following

$$\begin{aligned} x_s &= 2x_0 + q_s(x_0, 0)T_s \\ &= \pm 3 + \left(0.3 + 0.7 \sin\left(\frac{2\pi}{3}\left(\pm \frac{3}{2}\right)\right)\right) \frac{15}{7\pi} = \pm 3 + \frac{9}{14\pi}. \end{aligned} \quad (4.145)$$

Following [122], it is considered that the solution of equation (4.137) with initial condition in equation (4.138) develops discontinuities when $T > 5/\pi^2$. Moreover, the equation (4.139) is used to obtain the exact solution at a general position (x, y) for $t < \frac{0.5}{\pi^2}$ (when the solution is still smooth), and on the path s (equation (4.140)) for $t < \frac{15}{7\pi}$. To obtain the solution for $t \geq T_s$, with T_s the time that discontinuities develop, one may use the method of characteristics to update the location of the shock and the solution can be computed using the Riemann method (see e.g. [75]). However, we do not pursue this approach in this thesis. The non-smooth solution of the Burgers equation is obtained using the employed numerical schemes.

Table 4.3: Accuracy study for MUSCL, and multidimensional WENO3 reconstruction schemes, using 2D Burgers' equation results obtained at $T = 0.5/\pi^2$.

MUSCL			WENO3	
h	L^1 error	order	L^1 error	order
$\frac{3}{10}$	8.31E-04	-	8.18E-04	-
$\frac{3}{20}$	3.73E-04	1.1573	3.42E-04	1.26
$\frac{3}{40}$	1.04E-04	1.8378	9.23E-05	1.89
$\frac{3}{80}$	3.09E-05	1.7561	2.02E-05	2.19
$\frac{3}{160}$	8.58E-06	1.8475	2.18E-06	3.21
$\frac{3}{320}$	2.26E-06	1.93	3.09E-07	2.82

Numerical simulations have been carried out using the MUSCL scheme, and the multidimensional WENO3 reconstruction scheme. The time discretization is performed using the three-stage third-order accurate TVD Runge-Kutta scheme (section 4.3.6). Equation (4.137) is first integrated in time until the final time $T = 0.5/\pi^2$, when the solution is smooth, using a CFL number with $\mathcal{C} = 0.1$. Note that we take CFL relatively small such that it suits for the time integration for the coarsest to the finest grids, when the final time T is small. A grid convergence study is performed for this case in order to assess the performance of the employed discretization schemes for nonlinear problems in two dimensions. In Table 4.3 the results for the L^1 error norm and the accuracy are presented. Note that the order of accuracy of these numerical schemes is obtained only for the smooth parts of the numerical solution. When the numerical solution is non-smooth, the accuracy of the schemes reduces to first order accurate near discontinuities. This may also reduce the global accuracy of the solution to first order accurate.

Then, equation (4.137) is integrated further in time, first until $T = \frac{15}{7\pi}$ (when discontinuities develop on path s), and finally until $T = \frac{60}{7\pi}$, using a CFL number with $\mathcal{C} = 0.6$. Note that we increase the CFL number (compared to the one used in the preceding part) in order to speed up the computations.

The multidimensional WENO3 reconstruction results are presented in Figure 4.7, which are obtained using a computational grid with $[N_x \times N_y] = [80 \times 80]$, where N_x and N_y are the number of cells in x and y directions, respectively. Figures 4.7a, 4.7b, and 4.7c show the plots for $T = 0.5/\pi^2$, $T = 15/7\pi$, and $T = 60/7\pi$, respectively. Furthermore, Figure 4.7d shows the solution q along the path s (equation (4.140)) at $T = 15/7\pi$. The results clearly show that the results of the multidimensional WENO3 scheme have a good sharpness near the discontinuities in the solution.

Figure 4.7: multidimensional WENO3 reconstruction results for 2D Burgers' equation: (a) at $T = 0.5/\pi^2$; (b) at $T = 15/7\pi$; (c) at $T = 60/7\pi$; (d) plots along the path $s : x = y$ at $T = 15/7\pi$ compared to the exact solution.

RESULTS

In this chapter numerical simulations of unsteady cavitation problems for inviscid and turbulent compressible flow are presented. The numerical simulations are carried out using the framework described in chapter 4 to solve the URANS equations. Furthermore, the evaluation of the thermodynamic relations is carried out utilizing precomputed multiphase thermodynamic tables, using the developed POITC data interpolations, described in chapter 3. The employed turbulence models include the Menter SST, and the S-A models. Eskilsson & Bensow [26] showed that, when using the S-A model for the sheet cavitation problem, the predicted behavior of the shedding of the vapor cavities is inaccurate. They also showed that, compared to results from the S-A model, the results from the Menter SST model are much more accurate. In this thesis only the results that are obtained using the Menter SST model are presented.

The spatial discretizations are performed using different reconstruction schemes, which include the MUSCL scheme, the WENO scheme, the maximum principle-preserving WENO scheme, and the developed positivity-preserving WENO scheme. The inviscid fluxes are computed using the AUSM+_{up} for all speeds approximate Riemann solver, and for some numerical experiments using the HLLC-AUSM flux scheme. For the time discretization, the three-stage third-order accurate TVD Runge-Kutta scheme is used. For cavitating flows, the time steps required by the employed time discretization scheme are extremely small. This is because the utilized equilibrium cavitation model takes into account the physics of the almost incompressible (liquid) flow as well as the compressible (vapor and mixture) flow, which are solved using the compressible flow approach. For such a flow the Mach number ranges from low values in the liquid (low-Mach number flow), with a large value of the speed of sound c (e.g. $c \approx 1500 \text{ m s}^{-1}$), to relatively high values of the Mach number in the mixture, i.e. with low values of the speed of sound (e.g. with $c < 1 \text{ m s}^{-1}$, based on the acoustic speed of sound formulation). Therefore, in order to resolve the dynamics of the pressure waves, which are directly related to the quantity ρc (see e.g. [113]), and to satisfy the appropriate CFL condition for numerical stability, in particular for low-Mach number flow, the time step that is allowed is extremely small. In order to increase the time step, one may consider using implicit schemes such as the dual time integration scheme.

This chapter is organized as follows. First, the test case of 1D cavitating flow in expanding waves of Saurel *et al.* [108] is considered. Then, solutions of sheet cavitation on a 2D NACA0015 at 6 deg AOA are presented for inviscid flow as well as turbulent flow. The initial solution for this problem is obtained using the fully-wetted steady flow solution. Finally, this chapter ends with presenting results for numerical simulations

of vortex cavitation in the turbulent flow about Arndt's 3D elliptic hydrofoil, with a NACA66₂ – 415 profile, at 7 deg AOA.

5.1 1D cavitating flow in expanding waves

Considered is the test case of one-dimensional (1D) cavitating flow in expanding waves due to Saurel *et al.* [108]. In this study, the conditions and specifications used by Koop [68] are adopted. Initially there is water at rest in a tube with a length of L . A diaphragm in the middle of the tube separates the fluids in the two sections of the tube. At time t_0 , the diaphragm is removed and the fluids on the left and right side of the diaphragm are pulled apart with a velocity of u_0 in different directions (see Figure 5.1). Consequently, cavitation is initiated in the middle of the tube.

In the first subsection, MUSCL results, which are obtained using POITC as well as conventional non-POITC data interpolations are compared to show the need for using the POITC approach. For the remainder of the test cases in this chapter the POITC approach is utilized. In the next subsection, the results that are obtained using the scaling-limiter maximum principle WENO scheme, as well as the developed positivity-preserving WENO scheme are presented.

5.1.1 Results from MUSCL scheme, comparing POITC and non-POITC approach

Results of the numerical simulations are presented for 1D cavitating flow in expanding waves in a tube with a length of $L = 1\text{ m}$, with $u_0^L = -10\text{ m s}^{-1}$ and $u_0^R = 10\text{ m s}^{-1}$ at the left and right side of the diaphragm, respectively. The initial conditions for this test case are given in Table 5.1. The value of the cavitation number $\sigma \approx 1.72$ is computed from $\sigma = \frac{p_0 - p_v}{1/2 \rho_0 u_0^2}$ using the values given in Table 5.1, and with $p_v \approx 4254\text{ Pa}$.

The results are obtained using the MUSCL reconstruction scheme in combination with the HLLC-AUSM flux scheme. Note that similar results are obtained using the AUSM+-up flux scheme. For this test case we choose the HLLC-AUSM because, compared to the AUSM+-up, it allows taking larger time steps. Moreover, the three-stage third-order accurate TVD Runge-Kutta time integration scheme is employed. The numerical results are computed using 100 uniform grid cells, and the time step is chosen such that the CFL number $\mathcal{C} = 0.3$. The simulation is run up to a final time of $T = 2.4 \times 10^{-4}\text{ s}$. In order to characterize the thermodynamic state of the system, multiphase thermodynamic tables using the developed POITC data interpolations approach are employed. Moreover, in order to assess the performance of the POITC approach and to illustrate the issues with the conventional non-POITC approach, the results for the non-POITC approach are also presented, all at the time $T = 2.4 \times 10^{-4}\text{ s}$.

Figure 5.1: A schematic of cavitating expanding waves tube.

Table 5.1: Initial conditions for the 1D cavitating expanding waves, standard case.

$ u_0 $ [m s^{-1}]	p_0 [10^5 Pa]	T_0 [K]	ρ_0 [kg m^{-3}]	c_0 [m s^{-1}]	σ [—]
10	0.9	303.15	995.6	1539.6	1.72

Figure 5.2: Results for 1D cavitating expanding waves at $t = 2.4 \times 10^{-4} \text{ s}$ using MUSCL scheme, and multiphase thermodynamic tables using POITC approach ($\square$), as well as conventional non-POITC approach ($\circ$) for the tabular data of similar resolution, and for the analytically computed thermodynamic variables ($+$): (a) vapor void fraction; (b) velocity; (c) pressure; (d) speed of sound.

Figure 5.2 shows the results for the POITC and the conventional non-POITC approach for the tabular data of similar resolution, as well as the results of the simulations based on the analytically computed thermodynamic relations. Figure 5.2a shows the vapor void fraction. From this figure no apparent distinction is seen between the plots of the different approaches. However, note that the difference can become more apparent in other cases or in two-dimensional and three-dimensional simulations. Figure 5.2b shows the velocity. In this figure also the difference between the plots is not clearly visible. However, from a

Figure 5.3: Results for 1D cavitating expanding waves at $t = 2.4 \times 10^{-4}$ s using MUSCL scheme. Relative errors between the results obtained using interpolated data from thermodynamic tables, and the ones obtained using analytically computed thermodynamic variables. POITC approach ($\square$), and conventional non-POITC approach ($\circ$): (a) relative errors for pressure; (b) relative errors for speed of sound.

magnified view, shown at the right side of the figure, it can be seen that there is a slight difference in the results. In Figures 5.2c and 5.2d the pressure and speed of sound are presented, respectively. In these figures, the plots based on the POITC approach have negligible differences compared to the ones computed using the analytical thermodynamic approach. Furthermore, these results are similar to the results of Koop [68], who also used the analytic thermodynamic relations. However, the results for the simulations obtained using the conventional non-POITC approach show large deviations relative to the ones obtained based on the POITC approach, and the analytical thermodynamic approach. Moreover, note that these plots are obtained using the reconstruction of the component-wise variables. When characteristic-wise variables are used in the reconstruction procedure, the results are similar to the ones for the component-wise variables, and are therefore not shown.

In order to analyze these results, an accuracy study is performed. The relative errors of pressure and speed of sound that are obtained using POITC and non-POITC approaches are computed with respect to the pressure, and speed of sound obtained based on the analytical thermodynamic approach. The computed errors are shown in Figures 5.3a and 5.3b for the pressure and speed of sound, respectively. In these figures, the values of the relative errors of the results obtained using the conventional non-PIOTC approach (shown on the y -axis at the right side of the figures) are at most in $O(10^{-1})$ and $O(1)$ for pressure and speed of sound, respectively. In contrast, when using the PIOTC approach these errors are diminished to much lower values (shown on the y -axis at the left side of the figures), with maximum values of $O(10^{-4})$ and $O(10^{-3})$ for pressure and speed of sound, respectively.

In Figure 5.4 plots of results for the 1D cavitating expanding waves are presented at 4 moments in time. These plots are obtained using a characteristic-wise MUSCL scheme, the HLLC-AUSM flux scheme, and the multiphase thermodynamics tables using the POITC approach.

Figure 5.4: Results for 1D cavitating expanding waves at 4 times, using characteristic-wise MUSCL scheme and multiphase thermodynamic tables using POITC approach. $t_0 = 0$ s, $t_1 = 0.8 \times 10^{-4}$ s, $t_2 = 1.6 \times 10^{-4}$ s, and a final time of $t_3 = 2.4 \times 10^{-4}$ s: (a) vapor void fraction; (b) velocity; (c) pressure; (d) speed of sound.

Koop [68] has carried out numerical simulations of the same test case with the same number of grid cells, and using the component-wise MUSCL scheme, and HLLC-AUSM++ up for all speeds flux scheme. The results for the void fraction, velocity, and pressure in Figure 5.4 are similar to the results presented in [68]. Only, the plots of the speed of sound are to some extent different. The most likely reason for this difference is the characteristic-wise reconstruction of the variables used here (rather than the component-wise approach used in [68]), and the use of the HLLC-AUSM flux scheme rather than the flux scheme used in [68].

The presented results show that the numerical solution for this test case corresponds to two rarefaction waves running in opposite directions. In the rarefaction wave moving at a velocity equal to the speed of sound in the liquid, the pressure decreases rapidly from the initial pressure to the saturation pressure, here $p_{sat} \approx 4254$ Pa, but the vapor void fraction remains zero in the rarefaction wave. Over the rarefaction wave the velocity decreases 0.06 m s^{-1} . This corresponds to the perturbation from linear acoustic theory of $\Delta u \approx \frac{\Delta p}{\rho_0 c_0}$.

The vapor void fraction only changes at the interface (contact surface), where evaporation takes place at constant temperature and pressure. As the interface (liquid) moves away from the center of the tube vapor fills the void between the left-moving and right-moving liquid front. In between, the vapor void fraction equals 1.0. In the results of the numerical simulations the vapor is distributed over the grid cells. In Figure 5.4 the interface moves about $\frac{1}{4}\Delta x$ for the time $t_3 = 2.4 \times 10^{-4}$ seconds ($u_0 \times t_3 = 2.4 \times 10^{-3} = 0.24\Delta x$), so void fraction, α , becomes about 0.24 in the numerical simulation.

5.1.2 Results for positivity-preserving WENO scheme

Numerical simulations for 1D cavitating expanding waves using the higher-order accurate WENO scheme are presented. The tube has a length of $L = 6 \text{ m}$, the velocities at the left and right sides of the diaphragm are $u_0^L = -50 \text{ m s}^{-1}$ and $u_0^R = 50 \text{ m s}^{-1}$, respectively, and the initial conditions are given in Table 5.2. The value of the cavitation number $\sigma \approx 1.0$ is obtained from $\sigma = \frac{p_0 - p_v}{\frac{1}{2}\rho_0 u_0^2}$ with $p_v \approx 2321 \text{ pa}$, and using the values given in Table 5.2.

The employed spatial discretization schemes are the characteristic-wise MUSCL scheme, the fifth order accurate component/characteristic-wise WENO scheme denoted by WENO5 (without satisfying the maximum-principle property), the developed positivity-preserving WENO scheme with fifth-order accuracy denoted by log-WENO5, and the fifth order accurate Scaling Limiter (SL) maximum principle-preserving scheme [142] denoted by SL-WENO5.

Table 5.2: Initial conditions for the 1D cavitating expanding waves, increased-pressure case.

$ u_0 \text{ [m s}^{-1}\text{]}$	$p_0 \text{ [10}^5 \text{ Pa]}$	$T_0 \text{ [K]}$	$\rho_0 \text{ [kg m}^{-3}\text{]}$	$c_0 \text{ [m s}^{-1}\text{]}$	$\sigma \text{ [-]}$
50	12.5	293	996.13	1539.6	1.0

Figure 5.5: Results numerical simulation for 1D cavitating expanding waves using characteristic-wise MUSCL scheme (+) for reconstructed conservative variables, characteristic-wise SL-WENO5 (O) for reconstructed variables $Q = [\rho, u, e]^T$, and the developed positivity-preserving characteristic-wise log-WENO5 scheme (□) for reconstructed logarithmic variables $Q = [\ln(\rho), u, \ln(e)]^T$: (a) vapor void fraction; (b) density; (c) pressure; (d) velocity (e) speed of sound; (f) Mach number. $t = 1.6 \times 10^{-3}$ s.

Additionally, the inviscid fluxes are computed using the HLLC-AUSM flux scheme. Very similar results were obtained for the AUSM+-up for all speeds flux scheme. The time discretization is performed using the three-stage third-order accurate TVD Runge-Kutta scheme. The simulations are carried out using 600 uniform grid cells. A fixed CFL number $C = 0.3$ is chosen, and the solution is evolved until a final time of $T = 0.0016$ s.

Due to the occurrence of non-physical values of the density and/or the internal energy in the results for the WENO scheme, in which the positivity (or maximum principle) property is not preserved, the simulations using this scheme failed. In contrast, using the developed positivity-preserving log-WENO5 approach, as well as the maximum principle-preserving SL-WENO5 scheme the simulations could be carried out successfully.

The results are shown in Figure 5.5. The results from the MUSCL scheme are obtained using a characteristic-wise reconstruction of the conservative variables $\mathbf{q} = [\rho, \rho u, \rho E]^T$. The results of the log-WENO5 scheme, and the SL-WENO5 scheme presented in this figure are obtained using a characteristic-wise reconstruction of the semi-logarithmic primitive variables $\mathbf{Q} = [\ln(\rho), u, \ln(e)]^T$ with the components ρ and e as the target positivity-preserved variables. The target positivity-preserved variables ρ and e are taken as thermodynamically independent variables, thus, the SL-WENO5 scheme does not need any additional procedures to take into account the dependency of the target positivity-preserved variables. Afterwards the final reconstructed values at the cell faces are obtained using the exponential transformations of the reconstructed semi-logarithmic primitive variables. In order to perform the characteristic-wise reconstructions, and characteristic-wise logarithmic reconstructions, the approaches in Appendix A.2, and Appendix A.3 are pursued for the SL-WENO5 scheme, and the log-WENO5 scheme, respectively.

The results presented in Figure 5.5 show that the SL-WENO5 and the log-WENO5 results are similar, in particular for the pressure and speed of sound. Furthermore, it is observed that the results of the log-WENO5 scheme, and the SL-WENO5 scheme are less diffusive (with sharper gradients near discontinuities) than the results of the MUSCL scheme. Figures 5.5a and 5.5b are the plots of the vapor void fraction, and density, respectively, which show that the cavitation is well developed in the center part of the tube. Moreover, the magnified views in these figures show that the size of the cavity in the results of the MUSCL scheme is underestimated compared to the results from the log-WENO5 scheme, and the SL-WENO5 scheme, i.e. the results from the log-WENO5 scheme and the SL-WENO5 scheme for the density and void fraction are wider in the cavitating part of the tube. From a grid dependency study we observed that the results of the MUSCL scheme on the grids that are roughly 2.5 times finer than the current grid converged to the results from the log-WENO5 scheme, and the SL-WENO5 scheme in Figure 5.5.

5.2 Sheet cavitation on 2D NACA0015 at 6 deg AOA

Results of numerical simulations of unsteady sheet cavitation in the flow around the 2D NACA0015 hydrofoil at 6 deg AOA are presented. This is a standard test case in literature. It has also been considered by Sauer & Schnerr [107], Schnerr *et al.* [114], and Koop [68]. In contrast to the references just cited, tunnel walls have not been included, and nonreflecting boundary conditions are not used. Instead, a far-field boundary condition is used. Standard free-stream conditions used by Sauer & Schnerr [107], Schnerr *et al.* [114], and Koop [68] are a velocity of $U_\infty = 12 \text{ m s}^{-1}$, a pressure of $p_\infty = 0.9 \times 10^5 \text{ Pa}$, and a

Table 5.3: Free-stream conditions for cavitating inviscid flow around 2D NACA0015 hydrofoil at 6 deg AOA.

U_∞ [m s ⁻¹]	p_∞ [10 ⁵ Pa]	T_∞ [K]	ρ_∞ [kg m ⁻³]	c_∞ [m s ⁻¹]	σ [–]
50	12.5	293	998.7	1540.0	1.0

cavitation number of $\sigma = 1.0$. Following Koop [68], we use an alternative free-stream condition with a velocity of $U_\infty = 50 \text{ m s}^{-1}$. This velocity is taken higher than the standard conditions in order to speed-up the shedding process. However, the scaling law for dynamic similarity is obeyed when using the second type of the free-stream conditions, such that the cavitation number σ is kept the same as for the standard conditions. Hence, the free-stream pressure is increased to $p_\infty = 12.5 \times 10^5 \text{ Pa}$.

The numerical simulations are performed for both inviscid flow and for turbulent flow. The simulations for inviscid flow are carried out using structured and/or unstructured grids. For the turbulent flow simulations, hybrid grids consisting of structured grid cells in the near-wall region, and unstructured grid cells in remainder of the domain are used. The required thermodynamic variables are looked-up from precomputed multiphase thermodynamic tables using the developed POITC data interpolations approach. Furthermore, in order to assess the performance of the POITC approach and to demonstrate the issues with the conventional non-POITC approaches, results of the numerical simulations based on these methods are compared.

The initial conditions for the numerical simulation of unsteady flow can be taken as the uniform flow condition. However, when doing this initially the uniform flow reaches a solid wall (hydrofoil), and the problem becomes equivalent to solving a water hammer problem, which involves transient effects such as propagation of strong expansion and shock waves. Therefore, when using initialization with the uniform flow, a considerable amount of computational time is needed for the initial transient effects of the water hammer phase of the solution of the flow. To avoid this problem we use a steady fully-wetted steady flow around the hydrofoil as the initial condition for the simulation of the unsteady flow. This fully-wetted steady flow solution is obtained by using the modified Tait equation (see chapter 2) as the thermodynamic closure. Using this approach, the transient effects at the beginning of the simulations have already decayed in the initial steady flow solution, and the repeatable periodic shedding features of the cavitation are captured much faster.

The spatial discretizations are performed using the MUSCL scheme with a MinMod limiter for the structured grids and the Venkatakrishnan limiter for the unstructured as well as for the hybrid grids. Furthermore, for some numerical experiments the spatial discretizations are carried out using the multidimensional WENO scheme. In order to compute the inviscid fluxes the AUSM+-up for all speeds flux scheme is used. For the time discretization, the three-stage third-order accurate TVD Runge-Kutta scheme is employed.

Table 5.4: Free-stream conditions for cavitating turbulent flow around 2D NACA0015 hydrofoil at 6 deg AOA.

p_∞ [10^5Pa]	T_∞ [K]	ρ_∞ [kg m^{-3}]	M_∞ [–]	σ [–]	Re_∞ [–]
12.5	293	998.7	0.0325	1.0	6.46×10^6

5.2.1 Initial fully-wetted steady flow solution

Numerical simulations of steady flow solution of fully-wetted water flow around the 2D NACA0015, with chord length of $l = 0.13\text{ m}$, at 6 deg AOA for inviscid and turbulent flow fields are presented. The free-stream conditions are presented in Tables 5.3 and 5.4, for inviscid flow, and turbulent flow, respectively. For the turbulent flow, the free-stream velocity is $U_\infty = 50\text{ m s}^{-1}$. The free-stream velocity for inviscid flow, and turbulent flow is taken higher than the standard conditions (to speed up the simulations). Following the scaling law the free-stream pressure is also increased, such that the cavitation number is kept the same as for the standard conditions, i.e. $\sigma = 1.0$. By increasing the free-stream velocity, the free-stream Reynolds number is also increased. However, it is expected that the effect of this difference in Reynolds number on the cavitation number is marginal.

Based on the employed equilibrium cavitation model described in section 2, the Tait equation (see section 2.4.2) is used as the thermodynamic closure in order to obtain the wetted-flow solution. The space discretization is carried out using the MUSCL scheme with the MinMod limiter for structured grids and with the Venkatakrishnan limiter for the unstructured and hybrid grids. Furthermore, the AUSM+-up for all speeds numerical flux scheme is used to compute the inviscid fluxes. For the time discretization, the third-order accurate three-stage TVD Runge-Kutta method is employed by using a local time stepping approach.

Results for inviscid flow

Results of inviscid flow numerical simulations of fully-wetted steady flow of water about NACA0015 hydrofoil test case are presented. The free-stream conditions are given in Table 5.3. The numerical simulations have been carried out for O-type computational grids with farfield boundaries placed about 2000 chord lengths away from the hydrofoil, and the resolution of the grid at the farfield is taken several orders of magnitude coarser than the finest grid near the hydrofoil.

Two types of grids with different resolutions are considered, which are shown in Figure 5.6. The first grid, shown in Figure 5.6a, has a rather coarse resolution, with 128 cells around the hydrofoil and 36 cells in the normal direction. The second grid (Figure 5.6b) is relatively fine, it consists of 512 cells around the hydrofoil and 96 cells normal to the hydrofoil. For these grids, the resolution of the grid in the farfield is approximately 10^9 times larger (with respect to average cell area) than the resolution of the grid around the hydrofoil. We assume that the location of the farfield in combination with the coarse resolution of the grid in the farfield is sufficient to dissipate the flow

Figure 5.6: Details of O-type computational grid around 2D NACA0015 hydrofoil, with chord length $l = 0.13$ m, at 6 deg AOA used for inviscid flow simulations: (a) coarse grid with 128 cells around the hydrofoil and 36 cells normal to the hydrofoil; (b) fine grid with 512 cells around the hydrofoil and 96 cells normal to the hydrofoil.

disturbances.

The results for the fine grid are presented in Figure 5.7. In Figure 5.7a the flow field distribution of the Mach number is shown. Furthermore, in Figure 5.7b the flow field distribution of the negative of the pressure coefficient C_p is shown. In the areas in which $\sigma \leq -C_p$ (with $\sigma = 1.0$ for this test case), we have

$$\frac{p_\infty - p_v}{1/2\rho_\infty U_\infty^2} \leq -\frac{p - p_\infty}{1/2\rho_\infty U_\infty^2} \Rightarrow p \leq p_v. \quad (5.1)$$

This indicates that in these areas the pressure has reached values equal to or lower than the saturation vapor pressure, and thus cavitation is triggered. From Figure 5.7b the location of the stagnation point at $C_p = 1$ is visible. Moreover, it is observed that the highest values of $-C_p$ are obtained at the suction side of the hydrofoil just downstream of the stagnation point, where cavitation is expected to start.

Furthermore, in Figures 5.8a and 5.8b the surface distribution of $-C_p$ and the Mach number are presented, respectively, on computational grids with coarse-grid and fine-grid resolutions. From these figures it is observed that for the grid consisting of 512 cells around the hydrofoil, the results are similar to the results obtained on a 4 times coarser grid. Moreover, the results for the finest grid (with 512 cells around the hydrofoil) are rather close to the ones for a grid that is 2 times coarser (not presented here). Therefore, for the grid with 512 cells the pressure coefficient and Mach number are considered grid converged. The results in Figure 5.8 show the stagnation point ($C_p = 1$, $M = 0$) on the lower surface, close to the leading edge. Also the suction peak is on the upper surface just downstream of the leading edge. Here the pressure has a minimum and the velocity has a maximum.

Figure 5.7: Steady fully-wetted inviscid flow solution about NACA0015 at 6 deg AOA, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, using computational grid consisting of 512 cells around the hydrofoil and 96 cells normal to the hydrofoil: (a) solution for Mach number; (b) distribution of negative of pressure coefficient C_p .

Figure 5.8: Surface pressure and Mach number distribution, steady fully-wetted inviscid flow solution for NACA0015 at 6 deg AOA, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, using grids with 128 cells (○) and 512 cells (□) around the hydrofoil, respectively, and with 36 and 96 cells normal to the hydrofoil, respectively: (a) solution for negative of pressure coefficient C_p vs. non-dimensionalized position x/l with l the chord length; (b) solution for Mach number M vs. non-dimensionalized position x/l .

Results for turbulent flow

Results of numerical simulations for steady flow solution of turbulent flow of water around the NACA0015 hydrofoil are presented. The free-stream conditions are given in Table 5.4. The numerical simulations have been performed using the RANS equations with the Menter SST closure model on a hybrid grid with farfield boundaries placed 900 chord lengths away from the hydrofoil. For the presented grids, the ratio of the average value of the grid cell area in the farfield to that around the hydrofoil is approximately 10^{14} , which, in combination with the location of the farfield, is assumed to be sufficient to dissipate the flow disturbances at the farfield.

The hybrid grid is shown in Figure 5.9. The grid consists of about 50,000 cells with a very fine resolution near the hydrofoil in order to take into account the boundary layer. Results are presented in Figure 5.10. In Figure 5.10a the distribution of the dimensionless wall distance, y^+ , along the hydrofoil is shown. The definition of y^+ is given by

$$y^+ = \frac{u_* y}{\nu}, \quad (5.2)$$

where, $u_* = \sqrt{\frac{|\tau_w|}{\rho}}$ denotes the friction velocity, with τ_w the wall shear stress, y the distance to the nearest wall, and ν the local kinematic viscosity. For this grid, it is observed that the maximum value of y^+ is approximately 7. This occurs close to the leading edge, in the region of high values of the skin friction.

Figure 5.9: Details of hybrid (structured-unstructured) O-type computational grid around 2D NACA0015 hydrofoil with chord length $l = 0.13$ m for numerical simulations of turbulent flow, views of: (a) unstructured part of the grid; (b) structured-unstructured part of the grid around the hydrofoil.

Figure 5.10: Steady fully-wetted turbulent flow solution about NACA0015 at 6 deg AOA, $Re_\infty = 6.46 \times 10^{-6}$, $p_\infty = 12.5 \times 10^5 \text{Pa}$, obtained using RANS equations with Menter SST closure model: (a) distribution of y^+ along the surface of the hydrofoil (b) distribution of skin friction coefficient at the surface of the hydrofoil (c) solution for Mach number; (d) negative of pressure coefficient C_p distribution; (e) ratio of eddy viscosity to molecular viscosity, i.e. $\frac{\hat{\mu}}{\mu}$; (f) solution of $-C_p$ coefficient on the surface of the hydrofoil.

Figure 5.10b shows the solution for the skin friction coefficient, C_f , along the surface of the hydrofoil. The definition of the C_f is given by

$$C_f = \frac{|\tau_w|}{\frac{1}{2}\rho_\infty U_\infty^2}, \quad (5.3)$$

where, τ_w is the wall shear stress, and ρ_∞ , and U_∞ denote the free-stream density and pressure, respectively. The highest values of $C_f(x/l)$ occur in the region where the flow velocity is highest, i.e. on the upper surface around the point of minimum pressure. In Figure 5.10c the field distribution of the Mach number is depicted. Clearly this fully-wetted steady flow solution is a low-Mach number flow, with highest Mach number around 0.05, corresponding to a velocity of about 75 m s^{-1} . In Figure 5.10d distribution of the negative of the pressure coefficient C_p is shown. It is observed that along the suction side of the hydrofoil, in particular close to the leading edge, the values of $-C_p$ are larger, in which cavitation is expected to occur.

Figure 5.10e shows the ratio of the turbulent (eddy) viscosity to the dynamic (molecular) viscosity, i.e. $\frac{\hat{\mu}}{\mu}$. This figure shows larger values of the eddy viscosity in the boundary layers, specifically the boundary layer along the suction side. In the wake of the hydrofoil the region with appreciable values of $\hat{\mu}$ rapidly spreads cross-flow direction. Finally, in Figure 5.10f the solution for the $-C_p$ coefficient along the surface of the hydrofoil is presented. The differences with the pressure distribution for inviscid flow are that the suction peak is slightly lower and near the trailing edge effects of viscous flow are apparent, i.e. the stagnation type of flow for inviscid flow becomes a viscous trailing edge flow in which the flow separates tangential to the pressure side while along the upper side the pressure is somewhat lower due to curvature of the flow.

The employed grid is considered to be fine enough to perform the wetted flow and unsteady simulations, Although, the author realizes that the interaction between cavitation and the boundary layer in the near-wall region of the hydrofoil are complicated.

5.2.2 Results for inviscid cavitating flow using MUSCL scheme

Results for the numerical simulations of unsteady inviscid flow with sheet cavitation around the 2D NACA0015 hydrofoil, with chord length of $l = 0.13 \text{ m}$, at 6 deg AOA are presented. The free-stream conditions are given in Table 5.3, which correspond to a cavitation number $\sigma = 1$. For the initial conditions, the numerical simulations are restarted from the fully-wetted steady flow solution. The closure thermodynamic relations are looked-up from the precomputed multiphase thermodynamic tables and using the developed POITC interpolation procedure (see section 3). The space discretization is carried out using the MUSCL scheme with the MinMod limiter. The inviscid fluxes are computed using the AUSM+-up for all speeds scheme or the hybrid HLLC-AUSM scheme. For the time discretization, the third-order accurate three-stage TVD Runge-Kutta method is employed.

Results using POITC

Results for numerical simulations of sheet cavitation in inviscid flow about 2D NACA0015 hydrofoil at 6 deg AOA employing POITC are presented. The free-stream conditions corresponding to a cavitation number $\sigma = 1$ are given in Table 5.3. The AUSM+-up

for all speeds scheme is used to compute the inviscid fluxes. The computational grid is the O-type structured grid shown in Figure 5.6b, which consists of 512 cells around the hydrofoil and 96 cells normal to the hydrofoil. Based on the grid convergence study performed for the wetted-flow case in section 5.2.1, the resolution of the employed grid is considered to be also fine enough for resolving sheet cavitation, although, the author realizes that much more complicated physics is involved when cavitation occurs. Moreover, a time step of $t = 10^{-9}$ s is chosen such that all the physical phenomena associated in the unsteady cavitation can be captured. The computing time for 35 million time steps was approximately 670 hr, on 8 processors (Intel Xeon X5650 at 2.67 GHz).

Figure 5.11 shows the distribution of the void fraction at six different time instances. The increment between the time instances is 0.0005 seconds. The formation and shedding of the vapor cloud are clearly visible in these figures. Furthermore, the three time instances in the lower 3 figures in Figure 5.11 show the formation of the attached sheet cavity and the appearance of the re-entrant jet, leading to the formation of the next vapor cloud. When the vapor region, which contains vorticity, passes the trailing edge of the hydrofoil, vorticity of opposite sign is generated at the trailing edge, leading to a change in the force experienced by the hydrofoil. The vorticity at the trailing edge is so intense that the flow cavitates (last subfigure in Figure 5.11). In Figure 5.12, sequence of images of the pressure field is depicted. The time interval between these images is 10^{-5} seconds, that is, 50 times smaller than the time interval of the pictures shown in Figure 5.11.

It is clear that the thermodynamic cavitation model used in this thesis is able to predict the appearance and disappearance of the attached sheet cavity and the vapor cloud as well as the corresponding formation of pressure waves. Since the time interval between the pictures in Figure 5.12 are only 10^{-5} seconds, this shows that this phenomenon takes place at a much smaller time scale than the shedding of the vapor cloud. The region with high pressure is generated at the moment the shed vapor region disappears at a location just upstream of the trailing edge. Following the disappearance of the shed vapor, a shock wave is formed that propagates outward at high speed, estimated to be 3250 m s^{-1} .

A data analysis of the time history of the results is depicted in Figure 5.13. The plots are for the lift force denoted by F_Y and a nondimensionalized total vapor volume V_{tot} , which in 3D computational space is defined as follows:

$$V_{\text{tot}} = \frac{1}{l^3} \int_{\mathcal{V}} \alpha d\mathcal{V}, \quad (5.4)$$

and in 2D space it is determined from

$$V_{\text{tot}} = \frac{1}{l^2} \iint_{\mathcal{A}} \alpha d\mathcal{A}. \quad (5.5)$$

Here, l denotes the chord length of the hydrofoil, $\mathcal{V}$ and $\mathcal{A}$ denote the volume (in 3D space) and the area (in 2D space) of the computational domain, respectively, and α is the vapor void fraction.

Figures 5.13a, and 5.13b show the time history of V_{tot} and F_Y , respectively, starting from an initial time t_s . The plot for V_{tot} clearly indicates the periodicity of the unsteady shedding of vapor clouds. It shows a period of about 0.023 seconds (the wide window highlighted in Figure 5.13a) for the shedding of major vapor structures, and a fundamental shedding period of about 0.005 seconds (the narrow window highlighted in Figure 5.13a).

Figure 5.11: Distribution of the vapor void fraction at different time instances for the inviscid cavitating flow over 2D NACA0015 hydrofoil at 6 deg AOA, and $\sigma = 1$, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, fine grid (512×96 cells). Time increment 0.0005 seconds.

Figure 5.12: Distribution of the pressure at different time instances for the inviscid cavitating flow over 2D NACA0015 hydrofoil at 6 deg AOA, and $\sigma = 1$, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, fine grid (512×96 cells). Time increment 10^{-5} seconds.

Figure 5.13: Data analysis for part of the results for the 2D NACA0015 hydrofoil at 6 deg AOA with $\sigma = 1$, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, $\Delta t = 10^{-9} \text{ s}$, fine grid (512×96 cells): (a) time history of the dimensionless total vapor volume V_{tot} , with t_s the starting time; (b) time history of the lift force, F_Y ; (c) power spectrum of $V_{tot}(t)$, the frequency of unsteady shedding for major vapor structures, $f \approx 45 \text{ Hz}$ (solid circle symbol), the fundamental frequency of shedding, $f \approx 209 \text{ Hz}$ (solid square symbol); (d) power spectrum of $F_Y(t)$, the frequency of unsteady shedding is $f \approx 209 \text{ Hz}$.

This periodicity is not clearly visible when looking at the F_Y plot. However, the spectral analysis of the results using an FFT algorithm shows approximately equal fundamental frequency of shedding of $f \approx 209 \text{ Hz}$ for both the V_{tot} and F_Y plots. The FFT plots are presented in Figures 5.13c, and 5.13d for V_{tot} and F_Y , respectively. Also, in Figure 5.13c the shedding frequencies of 45 [Hz] (solid circle symbol), and 209 [Hz] (solid square symbol) corresponding to the the shedding of major vapor structures, and the fundamental shedding process, respectively, are specified.

The predicted fundamental frequency of shedding, i.e. $f \approx 209 \text{ Hz}$, is higher than the one predicted by Koop [68]. The most likely cause for this difference is the use of a far-field boundary rather than the tunnel-wall boundaries used in [68]. Moreover, note that in order to obtain the correct frequency of shedding, which corresponds to a repeatable vapor shedding behavior, the sampling time instances must be chosen after sufficiently

Figure 5.14: Data analysis of cavitating flow about 2D NACA0015 at 6 deg AOA with $\sigma = 1$, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, $\Delta t = 10^{-8} \text{ s}$, coarse grid (128×36 cells). Comparison of results numerical simulations employing POITC (solid line), and conventional non-POITC (dotted line) approach: (a) time history of the dimensionless total vapor volume $V_{tot}(t)$; (b) time history of the lift force, $F_Y(t)$; (c) power spectrum of V_{tot} ; (d) power spectrum of F_Y .

large number of time steps of the numerical simulations.

Comparing results of POITC and non-POITC approach

Results of numerical simulations for cavitating flow about 2D NACA0015 hydrofoil test case are presented for cases employing POITC and the conventional non-POITC approach (see section 3) using tabular data of similar size. The free-stream conditions are given in Table 5.3, which correspond to a cavitation number $\sigma = 1$. For these numerical simulations, the hybrid HLLC-AUSM flux scheme was employed, the coarse grid (consisting of 128×38 cells) shown in Figure 5.6a was used, and a time step of 10^{-8} seconds was chosen. In Figure 5.14 the data analysis of these simulations is presented.

Figures 5.14a, and 5.14b show the time history of the total vapor volume V_{tot} and the lift force F_Y . It is observed that the computed non-POITC V_{tot} and F_Y are rather

different from the ones obtained using the POITC approach. Not only are the phase and the amplitude of $V_{\text{tot}}(t)$ and $F_Y(t)$ different, but also the patterns observed in the results of the simulations using the POITC approach are not visible in the ones using the non-POITC approach. The spectral analysis of the results using the FFT algorithm for $V_{\text{tot}}(t)$ and $F_Y(t)$ are presented in Figures 5.14c, and 5.14d, respectively.

The values of the fundamental frequencies that are obtained using the POITC and non-POITC data for V_{tot} (Figure 5.14c) are $f = 162.56 \text{ Hz}$, and $f = 162.61 \text{ Hz}$, respectively. Figure 5.14d depicts the FFT results for F_Y . In contrast to the FFT results for V_{tot} , the FFT results for F_Y show more than one peak. The peak with the maximum value corresponds to the frequency of the shedding, and the remainder of the peaks mainly correspond to unsteady flow effects and the transient effects at the beginning of the simulations. For the results using the POITC approach, the value of the fundamental frequency from the FFT analysis of $F_Y(t)$ is $f = 162.56 \text{ Hz}$, which is approximately equal to the one for $V_{\text{tot}}(t)$. However, for the non-POITC case it appears that there are two fundamental frequencies in the FFT analysis of $F_Y(t)$. The values of these fundamental frequencies are $f_1 = 2.91 \text{ Hz}$, and $f_2 = 162.61 \text{ Hz}$. Furthermore, the maximum value of the power spectrum is obtained for the frequency of f_1 . Therefore, this data analysis also shows that when using the non-POITC method, besides the inaccurate solution of the problem for the field variables, the shedding frequency of the vapor is also predicted wrongly. It is noticed that the inaccuracy of the results of the non-POITC method is completely independent of the duration of the total time of the numerical simulations. Furthermore, it has been observed that the results using the non-POITC approach were also inaccurate for finer grid resolutions.

The reason for these inaccuracies in the results of the non-POITC method is that the large errors of the conventional non-POITC-based tables in the phase-transitioning regions (although only in a small part of the tables) are translated into computational errors in the entire computational domain.

Results showing the effect of reentrant jet

Numerical simulations of sheet cavitation in the flow around the NACA0015 at 6 deg AOA at different time instances, during a shedding cycle, employing POITC are presented. The free-stream conditions are given in Table 5.3, which correspond to a cavitation number $\sigma = 1$. Figure 5.15 shows the distribution of the vapor void fraction together with the streamlines in the flow. For these results the AUSM+-up for all speeds scheme was employed for computing the inviscid fluxes, the fine grid (consisting of 512×96 cells) shown in Figure 5.6b was used, and a time step of 10^{-9} seconds was chosen.

Figure 5.15a shows the shedding of a vapor cloud, which is formed in the previous shedding cycle. Furthermore, from the same figure it is observed that a sheet cavity is developing on the front part of the hydrofoil. The streamlines show the formation of vorticities, in particular in the area close to the trailing edge.

In Figure 5.15b, the sheet cavity is already developed, and from the streamlines it appears that a vortex behind the cavity is present, which shows that a reentrant jet moving upstream along the surface of the hydrofoil is about to detach the cavity from the hydrofoil. In Figures 5.15c, and 5.15d the reentrant jet splits off part of the sheet cavity, which turns into a vapor pocket moving downstream.

(a) $(t - t_0)/T = 0$ (b) $(t - t_0)/T = 0.3$ (c) $(t - t_0)/T = 0.5$ (d) $(t - t_0)/T = 0.7$ (e) $(t - t_0)/T = 0.8$ (f) $(t - t_0)/T = 1$

Figure 5.15: Distribution of vapor void fraction and streamlines at different time instances during a shedding cycle for the cavitating flow around 2D NACA0015 hydrofoil at 6 deg AOA, $\sigma = 1.0$, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, $\Delta t = 10^{-9} \text{ s}$, fine grid (512×96 cells), starting time t_0 , total time T .

Furthermore, the streamlines show that near the trailing edge of the hydrofoil interacting vortices are present. In Figures 5.15e, and 5.15f the second part of the sheet cavity also detaches, and the vapor cloud close to the trailing edge is about to disappear completely.

5.2.3 Results for inviscid flow using multidimensional WENO scheme

Results have been obtained for numerical simulations of sheet cavitation in inviscid flow around the NACA0015 hydrofoil at 6 deg AOA employing POITC, and using the multidimensional WENO reconstruction. These results, at simultaneous time instances, are compared to the results obtained using the MUSCL scheme. The free-stream conditions are given in Table 5.3, which correspond to a cavitation number $\sigma = 1$. For the initial conditions, the numerical simulations are restarted from the fully-wetted steady flow solution. The closure thermodynamic relations are looked-up from the precomputed multiphase thermodynamic tables and using the developed POITC interpolation procedure (see section 3). The inviscid fluxes are computed using the AUSM+-up for all speeds. For the time discretization, the third-order accurate three-stage TVD Runge-Kutta method is employed. A time step $\Delta t = 10^{-8}$ s is chosen. The coarse grid shown in Figure 5.6a is used. Using this coarse grid allows performing faster numerical experiments than for employing the fine grid.

Figure 5.16: Pressure field and superimposed vaporous regions (the areas inside the colored lines) at three time instances for the cavitating flow over 2D NACA0015 hydrofoil at 6 deg AOA, $\sigma = 1$, $U_\infty = 50 \text{ m s}^{-1}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, $\Delta t = 10^{-8} \text{ s}$, coarse grid (128×36 cells): (a) MUSCL scheme; (b) multidimensional reconstruction WENO3 (MutliD-WENO3) method.

Results for different time instances are shown in Figure 5.16. In Figure 5.16a results using the MUSCL method are depicted, and Figure 5.16b shows results using the third order accurate multidimensional WENO method, denoted by MultiD-WENO3. The figures show the pressure distribution, and superimposed vapor regions.

From these figures, it is clearly observed that the MultiD-WENO3 method predicts more dynamics compared to the MUSCL method. In particular, for the second and third time instances in Figure 5.16b the results of the MultiD-WENO3 method show the appearance of a pressure wave close to the leading edge, where the sheet cavity is split. However, for the simultaneous time instances, the MUSCL method does not predict the dynamics that are visible in the results from the MultiD-WENO3. These results demonstrate the potential of using higher-order methods for numerical simulations of cavitating flows. However, it should be noticed that when using the WENO (or similar higher-order) scheme for solving a cavitating flow problem involving strong discontinuities one needs to use a scheme that is maximum-principle preserving.

5.2.4 Results for turbulent flow using MUSCL scheme

Numerical simulations are presented for turbulent flow, with sheet cavitation, around the NACA0015 hydrofoil at 6 deg AOA using the MUSCL scheme. The employed equations of motion are the URANS equations with the Menter SST closure model.

The numerical simulations are restarted from the fully-wetted steady flow solution presented in section 5.2.1, which provides reasonable initial conditions. The free-stream conditions are given in Table 5.4 for a free-stream velocity of $U_\infty = 50 \text{ m s}^{-1}$ and increased pressure, such that the cavitation number is $\sigma = 1$. The thermodynamic quantities are obtained from the precomputed multiphase thermodynamic tables using the developed POITC interpolation procedure described in section 3. The spatial discretization of the inviscid fluxes is carried out using the MUSCL scheme with the Venkatakrishnan limiter, combined with the AUSM+-up for all speeds approximate Riemann solver. The viscous fluxes are computed using the values of the flow quantities and their gradients (which are evaluated using the Gauss method) at the cell faces. For the time discretization, the third-order accurate three-stage TVD Runge-Kutta method is employed. Furthermore, the scalar equations of the SST model are discretized using a first order accurate constant reconstruction scheme. The time discretization of these equations is performed using the implicit BDF1 scheme.

The computational grid is the hybrid grid shown in Figure 5.9, which consists of approximately 140,000 cells with a fine resolution around the surface of the hydrofoil designed to capture the boundary layer. For this grid the values of y^+ near the surface of the hydrofoil are close to unity with a maximum value of $y^+ \approx 7$. The computational time steps need to be taken rather small in order to capture all physical phenomena and to satisfy the appropriate CFL condition for performing stable numerical simulations. The employed computational time steps are smaller than $O(10^{-9})$ seconds.

The results at two sample time instance t_1 and t_2 of the simulations are shown in Figure 5.17. In Figures 5.17a and 5.17c the field pressure distribution is depicted and the corresponding vaporous region is indicated. Figure 5.17a shows that a sheet cavity is formed on the front part of the hydrofoil. In Figure 5.17c the sheet cavity is developed further along the surface of the hydrofoil, and a reentrant jet close to the front part of the hydrofoil is about to split off the cavity.

In Figures 5.17b and 5.17d the distribution of the ratio of the eddy viscosity to the molecular (dynamic) viscosity, i.e. $\frac{\hat{\mu}}{\mu}$, is presented. Comparing with the non-cavitating flow solution, Figure 5.10, shows that the sheet cavity results in increased levels of eddy viscosity above the aft part of the hydrofoil, though the maximum values in the flow field are of the same magnitude. Comparing with the results for the eddy viscosity at the time t_1 in Figure 5.17b, the development of the vapor cavity along the surface of the hydrofoil (Figure 5.17d) results in increased levels of the eddy viscosity around the interface of the cavity close to the trailing edge of the hydrofoil.

Figure 5.17: Results of numerical simulation of cavitating turbulent flow about 2D NACA0015 hydrofoil (with a chord length of $l = 0.13$ m) at 6 deg AOA, $\sigma = 1$, $Re_\infty = 6.46 \times 10^{-6}$, $p_\infty = 12.5 \times 10^5$ Pa, $\Delta t = 4 \times 10^{-11}$ s, hybrid grid (140,000 cells), at a sample time instance. Results are obtained using URANS equations with Menter SST model: (a),(c) Pressure field and superimposed vaporous region (the area inside colored line), time instances t_1 and t_2 ; (b),(d) ratio of eddy viscosity to dynamic viscosity, i.e. $\frac{\hat{\mu}}{\mu}$, time instances t_1 and t_2 .

5.3 Vortex cavitation Arndt's 3D elliptic hydrofoil at 7 deg AOA

Results of numerical simulations are presented for the turbulent flow with vortex cavitation about Arndt's 3D elliptic hydrofoil at 7 deg AOA (see Maines & Arndt [85], and Maines [83]). This hydrofoil with elliptic planform has a NACA66₂ – 415 profile shape in the symmetry plane with a root chord length of $l = 0.13\text{ m}$, and a span-wise length of $l_s = 0.15\text{ m}$. The hydrofoil geometry is shown in Figure 5.18. The elliptic planform of the hydrofoil is shown in Figure 5.18 (top). Figure 5.18 (bottom) shows the NACA66₂ – 415 cross-sectional profile.

A cavitation number of $\sigma = 1.0$ is used. The free-stream conditions are given in Table 5.5, which correspond to the case with a free-stream velocity of $U_\infty = 50\text{ m s}^{-1}$, and an elevated ambient pressure. For these free-stream conditions, the velocity and pressure are chosen at values higher than the standard conditions (keeping the cavitation number constant), in order to accelerate the computation of the cavitation cycles. By increasing the free-stream velocity, the free-stream Reynolds number is also increased, although, the effect on the cavitation is expected to be small. Furthermore, a far-field

Figure 5.18: Arndt's 3D elliptic hydrofoil, geometry of the hydrofoil, showing the elliptic planform (top), and NACA66₂ – 415 shape of the section in the symmetry plane (bottom).

Table 5.5: Free-stream conditions for cavitating turbulent flows about 2D NACA0015 hydrofoil at 6 deg AOA, and NACA66₂ – 415 elliptic hydrofoil at 7 deg AOA, increased-pressure case.

p_∞ [10^5Pa]	T_∞ [K]	ρ_∞ [kg m^{-3}]	M_∞ [–]	σ [–]	Re_∞ [–]
12.5	293	998.7	0.0325	1.0	6.46×10^6

boundary condition is used for the inflow/outflow conditions. The farfield boundary is located at about 50 chord lengths away from the hydrofoil. The grid resolution at the farfield is relatively coarse, i.e. approximately 10^{12} times larger (with respect to average cell volume) than the grid resolution at the tip of the hydrofoil. Here, it is assumed that the location of the farfield in combination with the coarse resolution of the grid in the farfield is sufficient to remove the flow disturbances at the farfield.

The initial solution for the unsteady compressible cavitating turbulent flow is the steady flow fully-wetted turbulent flow solution.

5.3.1 Initial fully-wetted steady flow solution

The fully-wetted steady flow solution of the water flow around Arndt's 3D elliptic hydrofoil, at 7 deg AOA is obtained for $Re_\infty = 6.46 \times 10^6$ and $M_\infty = 0.0325$. The free-stream conditions are given in Table 5.5. The space discretization is carried out using the MUSCL scheme with the Venkatakrishnan limiter, in combination with the AUSM+-up for all speeds numerical flux scheme for computing the inviscid fluxes. For the time discretization, the third-order accurate three-stage TVD Runge-Kutta method is employed using a local time stepping approach.

The results are presented in Figure 5.19. Figure 5.19a shows the grid on the surface of the hydrofoil as well as its plane of symmetry. Figure 5.19b shows the distribution of y^+ (see equation (5.2) for the definition) on the surface of the hydrofoil. For this grid, the value of y^+ has on most of the surface a value close to unity. However, it has a maximum value of $y^+ \approx 50$ at the tip. The distribution of the skin friction coefficient, C_f (see equation (5.3) for the definition), on the surface of the hydrofoil is depicted in Figure 5.19c. It shows the largest values of C_f at the tip of the hydrofoil close to the leading edge.

Figure 5.19d (left), and Figure 5.19d (right) show the distribution of the negative of the pressure coefficient, $-C_p$, at the pressure side and the suction side of the hydrofoil, respectively. In this figure, the flow direction is from left to right in Figure 5.19d (left), and vice versa in Figure 5.19d (right). From Figure 5.19d (left) it is observed that the stagnation pressure (at $C_p = 1.0$) occurs in the vicinity of the leading edge on the pressure side of the hydrofoil. Figure 5.19d (right) shows that on the suction side of the hydrofoil close to the tip, $-C_p$ reaches its maximum value. The figure also shows that in these areas close to the tip we have $\sigma = 1.0 \leq -C_p$. These are the areas where cavitation inception is expected to occur (see equation (5.1)).

Prior to running the unsteady flow simulations, it was checked whether or not the flow solution is indeed unsteady. Therefore, first the numerical simulations were performed using an approach for steady flow. It was observed that, when using this approach, the system showed an unsteady-like behavior. Hence, an approach for time-accurate simulation is pursued.

5.3.2 Results for cavitating flow

Results are presented for numerical simulations of the unsteady turbulent cavitating flow around Arndt's 3D elliptic hydrofoil, at 7 deg AOA. The free-stream conditions are given in Table 5.5, which correspond to a cavitation number of $\sigma = 1.0$, $Re_\infty = 6.46 \times 10^6$, and $M_\infty = 0.0325$. The spatial discretization is performed using the MUSCL scheme with

Figure 5.19: Steady flow solution fully-wetted turbulent flow around Arndt's 3D elliptic hydrofoil at 7 deg AOA, $\sigma = 1$, $\text{Re}_\infty = 6.46 \times 10^{-6}$, $p_\infty = 12.5 \times 10^5 \text{Pa}$: (a) computational grid consisting of approximately 2,000,000 cells; (b) distribution of y^+ ; (c) distribution of the skin friction coefficient; (d) distribution of negative of the pressure coefficient, C_p , at the pressure side (left), and the suction side (right).

the Venkatakrishnan limiter combined with the AUSM+-up for all speeds flux scheme to compute the inviscid fluxes. For the time discretization the three-stage third-order accurate TVD Runge-Kutta scheme is used employing a global time stepping approach. The time step needs to be taken extremely small (the reason for this is explained at the beginning of chapter 5), namely $O(10^{-11})$ seconds. In order to increase the time step, one may consider using the dual time integration approach or other implicit time integration schemes. However, the usage of the implicit time integration schemes for cavitation is not straightforward, and our efforts so far were not successful. The equations of the SST model are discretized using a first order accurate upwind scheme to compute

the convective scalar flux, and the time discretization is performed using the implicit BDF1 scheme.

Results are presented in Figure 5.20, which are obtained using the grid shown in Figure 5.19a. Furthermore, the distribution of y^+ on the surface of the hydrofoil using this grid for the steady flow fully-wetted solution is shown in Figure 5.19b. Figure 5.20a depicts the isosurface of $C_p = -0.5$ together with streamlines passing over the suction side. Figures 5.20b, 5.20c, and 5.20d show cross-flow planes with contours for static pressure, vorticity magnitude, and the ratio of the turbulent viscosity to the dynamic viscosity, i.e. $\frac{\bar{\mu}}{\mu}$, respectively. Furthermore, Figure 5.20e shows the distribution of the quantity Q colored with the vorticity magnitude. The Q -criterion is defined as [51]:

$$Q = \frac{1}{2} \left(|\Omega|^2 - |\mathbf{S}|^2 \right) > 0, \quad (5.6)$$

where, $\Omega_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)$, and $S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{partial x_i} \right)$ are the components of the

Figure 5.20: Continued, next page

(e) Isosurface $Q = 10^6 \text{ s}^{-2}$ colored with $|\omega|$

Figure 5.20: Results for numerical simulation of tip vortex cavitation in turbulent flow around Arndt's 3D elliptic hydrofoil at 7 deg AOA for $\sigma = 1.0$, $\text{Re}_\infty = 6.46 \times 10^{-6}$, $p_\infty = 12.5 \times 10^5 \text{ Pa}$, $\Delta t = 10^{-4} \text{ s}$: (a) isosurface of $C_p = -0.5$ and streamlines passing over suction side; (b) cross-flow planes with pressure iso-contours; (c) cross-flow planes with iso-contours vorticity magnitude; (d) cross-flow planes with iso-contours turbulent viscosity ratio $\frac{\mu}{\mu}$; (e) isosurface of at $Q = 1,000,000 \text{ s}^{-2}$ colored with vorticity magnitude.

vorticity tensor, and the rate-of-strain tensor, respectively. The Q-criterion defines a vortex in the regions in which $Q > 0$.

Figure 5.20a reveals the presence of the tip vortex through the swirling streamlines that are captured by this vortex. Note that the vortex core moves inward, first slightly upward and then downward with respect to the tip. This agrees with the results of vortex wake roll-up studies, e.g. Pullin [99]. Though, suggested by the swirling streamline patterns, that the vortex core is compact, the pressure distribution in Figures 5.20a and 5.20b show that the pressure inside the vortex core increases to values above $C_p = -0.5$ already a short distance downstream of the tip.

Experimental studies (e.g. see [83]) for similar flow conditions show that the tip vortex cavitates up to the farfield of the domain. This indicates that the pressure inside the core of the vortex is lower than the vapor pressure. This corresponds to a vortex that has a concentrated, compact distribution of vorticity. However, from the plots in Figure 5.20, in particular from Figure 5.20c it is observed that after a short distance downstream of the hydrofoil, the vorticity magnitude has decreased significantly. This results in a less compact vortex core, also clear from the distribution of Q in Figure 5.20e, with a static pressure that does not reach the low values required for cavitation to occur. The reason for this is mainly due to artificial dissipation that is introduced by the employed numerical approach, in particular the MUSCL reconstruction scheme enhanced by the turbulent eddy viscosity (Figure 5.20d). In order to improve the results one might use a finer grid, which is in particular refined downstream of the hydrofoil in the areas the vortex core that cavitation is expected to occur. This refined grid zone should extend to a large distance downstream of the hydrofoil.

CONCLUDING REMARKS AND FUTURE PROSPECTS

6.1 Conclusions

In the present work a computational method has been developed, which has been applied to predict the dynamics of sheet and vortex cavitation. For the equilibrium cavitation model developed by Saurel *et al.* [110], Schnerr *et al.* [114], Schmidt *et al.* [113], multiphase thermodynamic tables for all three phases, liquid, vapor, and mixture, have been presented.

The analytical expressions for the thermodynamic closure relations, which are computationally intensive (based on the approach in Koop [67]), were replaced by tables containing the same information. By splitting the tables in subtables, with equidistant spacing, an efficient look-up procedure has been obtained that requires hardly any computational time. Consequently, a speed-up of approximately a factor of 10 has been obtained compared to the original method by Koop [68]. However, due to a nonsmooth distribution of the data in the phase-transition regions of the multiphase tables, the conventional look-up procedures are inaccurate in these parts and therefore fail to provide a robust procedure with uniform accuracy for any thermodynamic table. To resolve this problem, the novel method of Phase-Oriented Interpolations in Transition Cells (POITC) has been developed. POITC significantly improves the uniformity of the accuracy of the multiphase tables and allows for preparing much more efficient multiphase tables. Accurate POITC tables occupy only about 400 MB of memory, whereas if prepared based on the conventional approaches they would occupy impractically large sizes of memory (hundreds of gigabytes) and still would not be as accurate in phase-transition zones.

The computational method has been assessed by carrying out 1D and 2D test cases for cavitating flows. The test case of 1D cavitating expanding waves has been performed using POITC, the conventional non-POITC interpolations, as well as the analytical thermodynamic expressions. The numerical simulations show a large deviation in results for the pressure and speed of sound that were computed based on the non-POITC interpolation from the ones computed based on the analytical thermodynamic relations. This is because the large errors of the conventional non-POITC-based tables in phase-transition regions (although they occupy only a small part of the tables) are translated into computational errors in the entire computational domain. However, it has been shown that when using the POITC interpolations the results were consistent with the ones based on the analytical thermodynamic relations. The difference between the results of the POITC approach and the ones of the analytical thermodynamic approach was so small that they could not be distinguished in the presented figures. The method has also been used to perform numerical simulations using the MUSCL-based schemes for the sheet cavitation

in the flow around the 2D NACA0015 at 6 deg AOA. In the results, the formation of the sheet cavity and the reentrant jet could clearly be observed, as well as the shedding and the disappearance of vapor regions. Furthermore, a comparison of the results based on the POITC and non-POITC approaches has been presented. Similar to the 1D test case, also in this case the results from the method using the non-POITC interpolations show large deviations from the results of the method using the POITC interpolations. The FFT data analysis of the time-dependent solution showed that the frequencies of the vapor shedding that were obtained using the data for the unsteady lift force and the time-dependent total vapor volume were inconsistent for the case of non-POITC interpolation, whereas they were consistent for the case of POITC interpolation. Furthermore, the fundamental frequency of vapor shedding for the non-POITC interpolation was different from the one for the case of POITC interpolation.

The constructed multiphase tables and the POITC interpolation in combination with the MUSCL scheme have been utilized to perform numerical simulations based on the URANS equations of tip vortex cavitation in the flow around Arndt's 3D elliptic hydrofoil. The results showed that, the numerically dissipative MUSCL family of schemes, in combination with the relatively small time steps in $O(10^{-11})$ seconds (required to resolve the physics of the problem and to satisfy the numerical stability), are not well-suited for an efficient and accurate simulation of flows involving vortex cavitation.

As alternative, more sophisticated approach based on the Weighted Essentially Non-Oscillatory (WENO) schemes has been considered. Preliminary results have been presented for the higher-order accurate multidimensional reconstruction WENO scheme applied to cavitating flow around the 2D NACA0015 hydrofoil, in which the discontinuities are not strong (no need to obey the maximum principle). However, when there are strong discontinuities in the flow field the scheme must obey a maximum principle. This is to avoid problems with the non-physical values in the flow field variables such as the density and/or internal energy, encountered due to rather small oscillations in the WENO solution of these variables. In this thesis, the non-limiting positivity-preserving log-WENO scheme has been developed for the finite volume WENO scheme in 1D space. The log-WENO scheme is rather simple, and it does not use any flux/slope limiter functions, i.e. no excessive numerical dissipation is introduced into the scheme. Through several numerical experiments the performance of the third order accurate log-WENO3 and fifth order accurate log-WENO5 schemes have been assessed.

The accuracy study of the log-WENO scheme showed that for the problems in which the transformed logarithmic variables have large gradients the accuracy of the scheme deviates from design accuracy, in particular when using a very fine resolution for the computational grid. Furthermore, the poor functioning of the smoothness indicators of the WENO scheme, when applied to the transformed logarithmic variables, has been identified as another potential cause for the deviation of the accuracy of the log-WENO scheme. The log+C-WENO has been developed to improve the accuracy of the log-WENO scheme. The log+C-WENO scheme, in which the transformed logarithmic variables have relatively small gradients, showed a better performance than the log-WENO scheme. For the log+C-WENO3 scheme, the expected third order accuracy has been retained. Furthermore, the L_1 norm of the errors of the log+C-WENO3 results were even smaller than the ones of the WENO3 results. Also, the log+C-WENO5 significantly improved the accuracy of the results compared to the log-WENO5. However, when the grid resolution was rather fine, the design accuracy of the log+C-WENO5 scheme was not achieved. It

is noticed that the log+C-WENO scheme has not been applied to the remainder of the test problems in this thesis. It has only been provided as a potential alternative to the original log-WENO scheme.

In the next test problem, the performances of the positivity-preserving log-WENO3 and log-WENO5 schemes for the reconstruction of the non-smooth density field inside isolated computational cells have been investigated. The results showed that when the WENO schemes did not obey the maximum principle or the positivity principle, the reconstructed density values became negative in some parts of the computational cell, in particular at the cell faces. In contrast, when using the developed positivity-preserving log-WENO scheme, and the maximum principle-preserving SL-WENO scheme, the positivity property of the density was preserved.

The positivity-preserving log-WENO scheme has also been applied to the system of equations in order to perform numerical simulations of 1D cavitating expanding waves. For this problem, in spite of the failure of the WENO scheme, which did not obey the maximum principle, the numerical simulations using the log-WENO scheme and the SL-WENO scheme have been carried out successfully. The log-WENO5 (fifth-order accurate) solution of the problem has been compared to the MUSCL results and the (fifth-order accurate) SL-WENO5 results. It has been shown that the positivity-preserving log-WENO5 results are numerically less dissipative (with a sharper solution near the discontinuities) compared to the MUSCL results. Furthermore, the log-WENO5 results were similar to the ones for the SL-WENO5 scheme.

6.2 Prospects

The following suggestions are proposed for future work on the numerical simulations of unsteady cavitating flows, in particular flows with vortex cavitation:

1. Investigate the effects of non-equilibrium phase change. The employed equilibrium cavitation model accounts for the non-equilibrium effects implicitly by using the assumption that cavitation inception occurs at $p = p_{sat}$, which is a reasonably good approximation for practical cases. However, using a cavitation model, which takes into account the non-equilibrium effects such as heat and mass transfer between the different phases of the flow, the effect of dissolved gas and impurities, etc, could provide a better insight into the physics of the problem and into the fundamental mechanisms of cavitation inception.
2. Investigate implicit time stepping techniques. In this thesis an explicit time integration scheme has been employed. The explicit schemes require extremely small time steps in order to resolve the physics of the cavitation patterns and to satisfy the numerical stability condition. Time steps of $O(10^{-11})$ seconds were used for carrying out the numerical simulations of the 3D tip vortex cavitation problem. On the other hand, a larger time step may be sufficient to capture the physics of the problem, in particular for the pressure waves. For example, the analysis of the solution of the sheet cavitation problem at different time instances showed that a time step of $O(10^{-6})$ seconds may be sufficient to represent the physics of the problem. If this is indeed the case, the implicit time integration methods will be significantly more efficient than their explicit counterparts. However, it

should be noticed that when higher order accurate WENO schemes are employed for the spatial discretization, using the implicit time integration schemes is not straightforward. An alternative to the implicit time integration schemes is the time accurate local time stepping approach (see e.g. Grote & Mitkova [39]), which is much better suited for WENO schemes.

3. In order to improve the results for the MUSCL-based numerical simulations of tip vortex cavitation, which were carried out in this thesis, one may consider using finer grid resolutions. Although, obtaining grid converged results for this problem is not straightforward, local grid refinement in the areas where vortex cavitation is expected could be beneficial.
4. Utilize the Large Eddy Simulations (LES) method for turbulent flow simulations of the tip vortex cavitation. The LES simulations could provide a better insight into the physics of unsteady cavitation. However, it is known that LES is rather sensitive to the amount of artificial dissipation in the numerical scheme. Therefore, when using the LES method it is important that the discretization schemes, in particular the spatial ones, are as less dissipative as possible. The types of the higher order accurate numerical schemes that do not use any slope/flux limiter functions are the ideal candidates for such schemes.
5. Extend the employed higher order accurate maximum principle- and positivity-preserving WENO schemes in 1D to multidimensions, in order to apply these schemes to 3D vortex cavitation (or similar) problems. The usage of the higher order accurate schemes, in which the amount of artificial dissipation is negligible, should significantly improve the efficiency and accuracy of the numerical simulations, in particular for the 3D vortex cavitation problem. To do so, one may use the maximum principle-preserving SL-WENO scheme. Furthermore, the positivity-preserving log-WENO scheme, which has been developed in this thesis, may be considered.

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Appendix $\mathcal{A}$

EIGENVALUE ANALYSIS

The 1D Euler equations in conservation form are given by

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = 0, \quad (\text{A.1})$$

where, $\mathbf{q}$ and $\mathbf{f}$ are the vectors of the conservative variables and the fluxes, respectively, with

$$\mathbf{q} = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u H \end{bmatrix}. \quad (\text{A.2})$$

Here, $E = e + \frac{1}{2}u^2$ and $H = E + \frac{p}{\rho}$ are the total specific energy and the total specific enthalpy, respectively. The equation (A.1) in quasi-linear form can be written as follows

$$\frac{\partial \mathbf{q}}{\partial t} + \underline{\underline{A}}_q \frac{\partial \mathbf{q}}{\partial x} = 0, \quad (\text{A.3})$$

where, $\underline{\underline{A}}_q = \frac{\partial \mathbf{f}}{\partial \mathbf{q}}$ is the Jacobian matrix. Considering a pair of independent variables (ρ, e) , i.e. density and internal energy, respectively, such that $p = p(\rho, e)$. This results in

$$\underline{\underline{A}}_q = \begin{bmatrix} 0 & 1 & 0 \\ \frac{\rho \left(\frac{\partial p}{\partial \rho} \right)_e - \rho u^2 + \left(\frac{1}{2}u^2 - e \right) \left(\frac{\partial p}{\partial e} \right)_\rho}{\rho} & \frac{u \left(2\rho - \left(\frac{\partial p}{\partial e} \right)_\rho \right)}{\rho} & \frac{\left(\frac{\partial p}{\partial e} \right)_\rho}{\rho} \\ u \left(\rho \left(\frac{\partial p}{\partial \rho} \right)_e + \left(\frac{1}{2}u^2 - e \right) \left(\frac{\partial p}{\partial e} \right)_\rho - \rho H \right)}{\rho} & \frac{\rho H - u^2 \left(\frac{\partial p}{\partial e} \right)_\rho}{\rho} & \frac{u \left(\rho + \left(\frac{\partial p}{\partial e} \right)_\rho \right)}{\rho} \end{bmatrix}. \quad (\text{A.4})$$

A.1 Conservative variables form of the Euler equations

A characteristic-wise decomposition of equation (A.3) gives

$$\frac{\partial \mathbf{w}}{\partial t} + \underline{\underline{A}} \frac{\partial \mathbf{w}}{\partial x} = 0, \quad (\text{A.5})$$

where $\underline{\underline{\Lambda}} = \underline{\underline{R}}_q^{-1} \underline{\underline{A}} \underline{\underline{R}}_q$ is the diagonal matrix of the eigenvalues, and $\partial \mathbf{w} = \underline{\underline{R}}_q^{-1} \partial \mathbf{q}$ are the difference of the transformed characteristic variables with $\underline{\underline{R}}_q$ and $\underline{\underline{R}}_q^{-1}$ the right and left eigenvector matrices, respectively. The following expressions for $\underline{\underline{\Lambda}}$ and $\underline{\underline{R}}_q$ are obtained:

$$\underline{\underline{\Lambda}} = \begin{bmatrix} u & 0 & 0 \\ 0 & u+c & 0 \\ 0 & 0 & u-c \end{bmatrix}, \quad \underline{\underline{R}}_q = \begin{bmatrix} \Theta_1 & \frac{1}{H+uc} & \frac{1}{H-uc} \\ u\Theta_1 & \frac{u+c}{H+uc} & \frac{u-c}{H-uc} \\ 1 & 1 & 1 \end{bmatrix}, \quad (\text{A.6})$$

where

$$\Theta_1 = \frac{\left(\frac{\partial p}{\partial e}\right)_\rho}{E\left(\frac{\partial p}{\partial e}\right)_\rho - \rho\left(\frac{\partial p}{\partial \rho}\right)_e}, \quad (\text{A.7})$$

and c is the acoustic speed of sound, which is defined as follows:

$$c = \frac{\sqrt{\rho^2 \left(\frac{\partial p}{\partial \rho}\right)_e + p \left(\frac{\partial p}{\partial e}\right)_\rho}}{\rho}. \quad (\text{A.8})$$

A.2 Primitive variables form of the Euler equations

Following the procedure in section 4.4.3 for transformation of the conservative variables to primitive variables, given the primitive variables $\mathbf{Q}$, the equation (A.3) can be rewritten as follows:

$$\frac{\partial \mathbf{Q}}{\partial t} + \underline{\underline{P}}_Q^{-1} \underline{\underline{A}} \underline{\underline{P}}_Q \frac{\partial \mathbf{Q}}{\partial x} = 0, \quad (\text{A.9})$$

where, $\underline{\underline{P}}_Q = \frac{\partial \mathbf{q}}{\partial \mathbf{Q}}$ is the transformation matrix. Furthermore, a characteristic-wise decomposition of equation (A.9) gives:

$$\frac{\partial \mathbf{w}_Q}{\partial t} + \underline{\underline{\Lambda}} \frac{\partial \mathbf{w}_Q}{\partial x} = 0, \quad (\text{A.10})$$

where, $\underline{\underline{\Lambda}} = \underline{\underline{R}}_q^{-1} \underline{\underline{A}} \underline{\underline{R}}_q$ (note that the eigenvalues are identical to the ones in equation (A.5)), and $\partial \mathbf{w}_Q = \underline{\underline{R}}_Q^{-1} \partial \mathbf{Q}$, with $\underline{\underline{R}}_Q^{-1}$ the matrix of the left eigenvectors of $\underline{\underline{P}}_Q^{-1} \underline{\underline{A}} \underline{\underline{P}}_Q$.

Different sets of primitive variables can be chosen for $\mathbf{Q}$. Some of these cases are described in the following.

Case 1:

Considering the primitive variables:

$$\mathbf{Q} = \begin{bmatrix} \rho \\ u \\ e \end{bmatrix}, \quad (\text{A.11})$$

and choosing the pair of independent variables (ρ, e) we get:

$$\underline{\underline{P}}_Q = \begin{bmatrix} 1 & 0 & 0 \\ u & \rho & 0 \\ E & \rho u & \rho \end{bmatrix}, \quad \underline{\underline{R}}_Q = \begin{bmatrix} \Theta_2 & \frac{\rho^2}{p} & \frac{\rho^2}{p} \\ 0 & \frac{\rho c}{p} & -\frac{\rho c}{p} \\ 1 & 1 & 1 \end{bmatrix}, \quad (\text{A.12})$$

where,

$$\Theta_2 = -\frac{\left(\frac{\partial p}{\partial e}\right)_\rho}{\left(\frac{\partial p}{\partial \rho}\right)_e}, \quad (\text{A.13})$$

and c is the acoustic speed of sound, which is defined in equation (A.8).

Case 2:

Considering the primitive variables:

$$\mathbf{Q} = \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}, \quad (\text{A.14})$$

and choosing the pair of independent variables (ρ, p) we get:

$$\underline{\underline{P}}_Q = \begin{bmatrix} 1 & 0 & 0 \\ u & \rho & 0 \\ E + \rho \left(\frac{\partial e}{\partial \rho}\right)_p & \rho u & \rho \left(\frac{\partial e}{\partial p}\right)_\rho \end{bmatrix}, \quad \underline{\underline{R}}_Q = \begin{bmatrix} 1 & \frac{1}{c^2} & \frac{1}{c^2} \\ 0 & \frac{1}{\rho c} & -\frac{1}{\rho c} \\ 0 & 1 & 1 \end{bmatrix}, \quad (\text{A.15})$$

where, c is the acoustic speed of sound, which is defined in equation (A.8). Note that a direct eigenvalue analysis, results in the following expression for the acoustic speed of sound:

$$c = \frac{\sqrt{\frac{p - \rho^2 \left(\frac{\partial e}{\partial \rho}\right)_p}{\left(\frac{\partial e}{\partial p}\right)_\rho}}}{\rho}. \quad (\text{A.16})$$

Multiplying the expression inside the square root by $\frac{\left(\frac{\partial p}{\partial e}\right)_\rho}{\left(\frac{\partial p}{\partial e}\right)_\rho}$ we get:

$$\frac{p - \rho^2 \left(\frac{\partial e}{\partial \rho}\right)_p}{\left(\frac{\partial e}{\partial p}\right)_\rho} = p \left(\frac{\partial p}{\partial e}\right)_\rho - \rho^2 \left(\frac{\partial e}{\partial \rho}\right)_p \left(\frac{\partial p}{\partial e}\right)_\rho \quad (\text{A.17})$$

Furthermore, using Maxwell's thermodynamic relations we have

$$\left(\frac{\partial e}{\partial \rho}\right)_p = -\left(\frac{\partial e}{\partial p}\right)_\rho \left(\frac{\partial p}{\partial \rho}\right)_e. \quad (\text{A.18})$$

Hence, using the equations (A.17) and (A.18), the expression for the acoustic speed of sound in equation (A.16) can be rewritten as follows:

$$c = \frac{\sqrt{p \left(\frac{\partial p}{\partial e} \right)_\rho - \rho^2 \left(- \left(\frac{\partial e}{\partial p} \right)_\rho \left(\frac{\partial p}{\partial \rho} \right)_e \right) \left(\frac{\partial p}{\partial e} \right)_\rho}}{\rho} = \frac{\sqrt{p \left(\frac{\partial p}{\partial e} \right)_\rho + \rho^2 \left(\frac{\partial p}{\partial \rho} \right)_e}}{\rho}, \quad (\text{A.19})$$

which is the same expression as equation (A.8).

A.3 Logarithmic variables form of the Euler equations

Given the conservative variables $\mathbf{q}$ in equation (A.2), we consider the logarithmically transformed primitive variables

$$\mathbf{Q} = \begin{bmatrix} \ln(\rho) \\ u \\ \ln(e) \end{bmatrix}. \quad (\text{A.20})$$

The characteristic-wise decomposition of equation (A.1) based on the logarithmic variables in equation (A.20) can be performed by pursuing the procedure presented in section A.2. Alternatively, one can use the characteristic-wise non-logarithmic variables and then transform them to the characteristic-wise logarithmic variables. This approach is described in the following.

We choose the set of primitive variables

$$\hat{\mathbf{Q}} = \begin{bmatrix} \rho \\ u \\ p \end{bmatrix}. \quad (\text{A.21})$$

Then we can rewrite equation (A.10) as follows:

$$\frac{\partial \hat{\mathbf{w}}_{\hat{\mathbf{Q}}}}{\partial t} + \underline{\underline{\Lambda}} \frac{\partial \hat{\mathbf{w}}_{\hat{\mathbf{Q}}}}{\partial x} = 0, \quad (\text{A.22})$$

where, $\underline{\underline{\Lambda}} = \underline{\underline{R}}_q^{-1} \underline{\underline{A}}_q \underline{\underline{R}}_q = \underline{\underline{R}}_{\hat{\mathbf{Q}}}^{-1} \underline{\underline{\hat{A}}}_{\hat{\mathbf{Q}}} \underline{\underline{\hat{R}}}_{\hat{\mathbf{Q}}}$, and $\partial \hat{\mathbf{w}}_{\hat{\mathbf{Q}}} = \underline{\underline{R}}_{\hat{\mathbf{Q}}}^{-1} \partial \hat{\mathbf{w}}_{\hat{\mathbf{Q}}}$, with $\underline{\underline{R}}_{\hat{\mathbf{Q}}}^{-1}$ the matrix of the left eigenvectors of $\underline{\underline{\hat{A}}}_{\hat{\mathbf{Q}}} = \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}}^{-1} \underline{\underline{\hat{A}}}_q \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}}$, with $\underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}} = \frac{\partial \mathbf{q}}{\partial \hat{\mathbf{Q}}}$ the transformation matrix. Therefore, for $\underline{\underline{A}}_q$ we have

$$\underline{\underline{A}}_q = \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}} \underline{\underline{\hat{A}}}_{\hat{\mathbf{Q}}} \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}}^{-1} = \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}} \underline{\underline{\hat{R}}}_{\hat{\mathbf{Q}}} \underline{\underline{\Lambda}}_{\hat{\mathbf{Q}}} \underline{\underline{\hat{R}}}_{\hat{\mathbf{Q}}}^{-1} \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}}^{-1}. \quad (\text{A.23})$$

Additionally, we can rewrite equation (A.1) in terms of the logarithmically transformed variables $\mathbf{Q}$ as

$$\frac{\partial \mathbf{Q}}{\partial t} + \underline{\underline{A}}_Q \frac{\partial \mathbf{Q}}{\partial x} = 0, \quad (\text{A.24})$$

where, $\underline{\underline{A}}_Q = \frac{\partial \mathbf{f}}{\partial \mathbf{Q}}$ is the Jacobian matrix with respect to $\mathbf{Q}$. Furthermore, we have $\underline{\underline{A}}_Q = \underline{\underline{P}}_Q^{-1} \underline{\underline{A}}_q \underline{\underline{P}}_Q$ (with $\underline{\underline{P}}_Q = \frac{\partial \mathbf{q}}{\partial \mathbf{Q}}$ the transformation matrix), which, using equation (A.23), can be rewritten as

$$\underline{\underline{A}}_Q = \underline{\underline{P}}_Q^{-1} \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}} \underline{\underline{\hat{R}}}_{\hat{\mathbf{Q}}} \underline{\underline{\Lambda}}_{\hat{\mathbf{Q}}} \underline{\underline{\hat{R}}}_{\hat{\mathbf{Q}}}^{-1} \underline{\underline{\hat{P}}}_{\hat{\mathbf{Q}}}^{-1} \underline{\underline{P}}_Q. \quad (\text{A.25})$$

Moreover, because $\underline{\underline{A}}_Q = \underline{\underline{R}}_Q \underline{\underline{\Lambda}} \underline{\underline{R}}_Q^{-1}$, the right and left eigenvectors matrices are computed from the following:

$$\underline{\underline{R}}_Q = \underline{\underline{P}}_Q^{-1} \hat{\underline{\underline{P}}} \hat{\underline{\underline{R}}}, \quad \text{and} \quad \underline{\underline{R}}_Q^{-1} = \hat{\underline{\underline{R}}}^{-1} \hat{\underline{\underline{P}}}^{-1} \underline{\underline{P}}_Q, \quad (\text{A.26})$$

and the characteristic-wise logarithmic variables are computed by $\partial \mathbf{w}_Q = \underline{\underline{R}}_Q^{-1} \mathbf{Q}$. The values of the matrices $\hat{\underline{\underline{P}}}$ and $\hat{\underline{\underline{R}}}$ (and their inverse matrices) are computed using equation (A.15), and the transformation matrix $\underline{\underline{P}}_Q$ is given by:

$$\underline{\underline{P}}_Q = \begin{bmatrix} \frac{1}{\rho} & 0 & 0 \\ -\frac{u}{\rho} & \frac{1}{\rho} & 0 \\ \frac{u-E}{\rho e} & -\frac{u}{\rho e} & \frac{1}{\rho e} \end{bmatrix}. \quad (\text{A.27})$$

Note that this procedure can also be performed using primitive variables $\hat{\underline{\underline{Q}}}$ different from the ones in equation (A.21).

Appendix $\mathcal{B}$

CONSISTENCY BETWEEN PRESSURE AND SPEED OF SOUND

In Chapter 2 it was shown that the Wallis [133] formulation in equation (2.41) for the speed of sound employed by the equilibrium cavitation model is not consistent with the acoustic speed of sound (equation (2.40)). Furthermore, since the acoustic speed of sound is slope discontinuous when transitioning from the mixture to the liquid phase (see Figure 2.2), it is not so straightforward to utilize the acoustic speed of sound formulation in numerical simulations (due to numerical instabilities). In this chapter a modified acoustic speed of sound formulation is sought, aiming to be consistent with the original formulation and to be used in numerical simulations in an efficient and numerically stable manner. From equation (2.40), it is observed that the acoustic speed of sound is dependent on pressure. Therefore, in order to obtain a consistent formulation, any modifications in the speed of sound must be consistent with the values of pressure that are used in equation (2.40) and vice versa.

B.1 Acoustic speed of sound expression: a PDE

The relation for the acoustic speed of sound based on the independent variables (ρ, e) is presented in equation (2.40). This relation can be rewritten as

$$\frac{\partial p}{\partial \rho} + \frac{p}{\rho^2} \frac{\partial p}{\partial e} = c^2. \quad (\text{B.1})$$

It is observed that this equation is actually a Partial Differential Equation (PDE). Furthermore, it is observed that the expression in equation (B.1) is similar to a 1D Burgers equation for a variable $q(x, t) \equiv p$, with $t \equiv \rho$, $x \equiv e$, and with a convection speed $f(q(x, t), t) = \frac{q}{t^2} \equiv \frac{p}{\rho^2}$, and a source term, given by

$$\frac{\partial q(x, t)}{\partial t} + f(q(x, t), t) \frac{\partial q(x, t)}{\partial x} = S(x, t), \quad (\text{B.2})$$

where $S(x, t) = c^2$ is the source (forcing) term. The solution of this equation for q (and thus p) can help us to understand the effects of an inconsistent speed of sound on the pressure. For example, using this equation we can compute the pressures corresponding to the speeds of sound obtained using the Wallis formulation. In order to solve the PDE in equation (B.2) we need to set the initial and boundary conditions for q . Furthermore,

we assume that the values of the source term $\mathcal{S}$ are known. One may seek an analytical solution for equation (B.2). Alternatively, a numerical approach using a finite volume, finite difference or similar scheme can be pursued. In this thesis we use a finite difference scheme to solve this equation.

Given the values of the Wallis speed of sound from equation (2.41), the corresponding values of pressure are plotted in Figure B.1, which are obtained by solving a simplified version of equation (B.1) using a finite difference numerical scheme. The simplified form is obtained by using a constant-temperature assumption, which results in an equation similar to a time evolution problem. In the same figure the plots of pressure based on the governing equations of the employed equilibrium cavitation model are also shown. These plots are obtained for a range of density with $0.005 \leq \rho \leq 1100 \text{ kg m}^{-3}$, and at a constant temperature of $T = 298 \text{ K}$.

Compared to the pressure curve of the equilibrium cavitation model, the Wallis-based pressure curve is rather smooth. However, from Figure B.1 it is observed that the magnitudes of pressure for the Wallis-based pressure curve are much higher than the equilibrium cavitation model. Moreover, it is noticed that for the Wallis-based pressure plots the cavitation inception occurs at much higher pressure compared to the equilibrium cavitation model. Additionally, the Wallis-based vapor pressure does not follow the vapor pressure curve of the equilibrium cavitation model. The reason for this is explained in the following. As mentioned before, the equation that is solved is similar to a time evolution problem. The initial condition for the pressure p in this problem is set to the liquid pressure value at $\rho = 1100 \text{ kg m}^{-3}$, and p is then evolved, using a finite difference approach, until its value at $\rho = 0.005 \text{ kg m}^{-3}$ is obtained. From Figure B.1 it is observed that the liquid Wallis-based pressure follows the equilibrium cavitation curve correctly, which shows that the initial condition is chosen correctly. In the mixture phase, the Wallis-based pressure curve is different from the equilibrium cavitation model, which is due to the difference between the expressions for c and thus p in these models. This results in a computed Wallis-based vapor saturation point, which is also different from the equilibrium cavitation model. Therefore, due to a shift in the saturated vapor point in the Wallis-based pressure curve, the computed values of p in the vapor phase do not follow the equilibrium cavitation curve. Because of these reasons, a Wallis-based formulation for pressure can lead to incorrect predictions of the physical phenomenon in cavitation, and is thus not considered in this thesis.

B.2 Smoothing out the curves

In this section, a smoothening of the acoustic speed of sound in the slope discontinuous regions is considered. Since, a consistent thermodynamic formulation is sought, any modification of the speed of sound must be consistent with the pressure based on equation (B.1). It is noticed that the data for pressure is also slope discontinuous in mixture-liquid phase-transitioning regions (see Figure 2.3). This is also the reason for the discontinuous acoustic speed of sound. Because of this and for the sake of consistency, we first smooth out the pressure curves. Then, the smoothened pressure should also result in a smooth acoustic speed of sound.

In order to smooth out a curve with slope discontinuous data, part of the data on the slope discontinuous region of the curve is recomputed using a blending function, such that the new part of the curve becomes smooth. Assuming that for the densities

Figure B.1: $p - v$ plots, with $v = 1/\rho$, in a logarithmic scale: pressure plots which are consistent with the Wallis speed of sound formulation (dashed curve), pressure plots of the equilibrium cavitation model (dash-dot curve), liquid and saturation curves (solid curve), and a magnified view of the pressure plots about the liquid saturation curve shown on the right side of the figure. The plots are obtained for $0.005 \leq \rho \leq 1100 \text{ kg m}^{-3}$, and $T = 298 \text{ K}$.

$\rho \in [\rho_{cut,1}, \rho_{cut,2}]$ we have a slope discontinuous data for the pressure $p \in [p_{cut,1}, p_{cut,2}]$, and considering that p increases monotonically with ρ , the following blending formula is employed to smooth out the data for pressure:

$$p_{sm} = \left(\frac{(1 - \beta_{sm})}{(p_{cut,1})^{1/2}} + \frac{\beta_{sm}}{(p_{cut,2})^{1/2}} \right)^{-2}, \quad (\text{B.3})$$

where β_{sm} is the blending coefficient given by

$$\beta_{sm} = \frac{\rho - \rho_{cut,1}}{\rho_{cut,2} - \rho_{cut,1}}. \quad (\text{B.4})$$

Furthermore, we consider that

$$\begin{cases} \rho_{cut,1} = 0.99\rho_{l,sat} \\ \rho_{cut,2} = 1.0005\rho_{l,sat} \end{cases}, \quad (\text{B.5})$$

Using the known values of $\{\rho_{cut,1}, \rho_{cut,2}\}$ the values of $\{p_{cut,1}, p_{cut,2}\}$ are then computed.

In Figure B.2 a plot of a smoothened pressure curve is presented which is obtained for a constant temperature of $T = 298 \text{ K}$, and for a density range of $0.005 \leq \rho \leq 1100$. In the same figure, the original non-smooth pressure curve is also included. It is observed that compared to the original non-smooth pressure curve, the newly obtained curve is rather smooth. However, for the smoothened pressure curve the liquid saturation point is shifted to a higher values of pressure. This is highly undesirable, because a cavitation inception occurring at such high pressures is not physical. Generally speaking we would like to

Figure B.2: $p - v$ plots, with $v = 1/\rho$, in a logarithmic scale: non-smooth pressure curve (line with circle points), smoothed pressure curve (line with triangle points), liquid and saturation curves (solid curve). The plots are obtained for the ranges of the variables with $0.005 \leq \rho \leq 1100 \text{ kg m}^{-3}$, $T = 298 \text{ K}$.

obtain a smooth curve, which is as close as possible to the original non-smooth curve. However, it is not straightforward to control all the parameters to obtain a smoothed curve with such properties. When using the function in equation (??), the smoother the curve gets the higher the value of the saturation pressure point becomes, and the more the smoothed curve gets close to the original non-smooth curve, the less smooth it becomes.

Using the formulation in equation (??), the constant temperature pressure curves are smoothed for a range of temperatures with $273.16 \leq T \leq 350 \text{ K}$, which are shown in Figure B.3a. In the same figure the shifted (liquid) saturation points for the smoothed curves are also specified. It is observed that for the highest temperature, i.e. $T = 350 \text{ K}$, the shift in saturation point is much less than that for the lowest temperature, i.e. $T = 273.16 \text{ K}$. This is not desirable in the numerical simulations. However, as mentioned before, it is impossible to obtain a curve which is smooth enough and at the same time very similar to the original non-smooth curve. Furthermore, in the same figure a magnified view of the liquid phase and part of the mixture phase is depicted. It is observed that other than the sharp gradients in the liquid-mixture phase-transitioning region, the gradients in the liquid phase (which are original and not smoothed) are also variant (this is not visible until the plots are zoomed in). These variations in liquid phase gradients also add to the difficulties in smoothing of the pressure curves. Additionally, for the modified regions in the smoothed pressure curves, the values of internal energy also need to be adapted (because in the smoothed regions the temperature is different from the original temperature in the non-smooth curves). However, we do not take into account this inconsistency for internal energy in the smoothed regions.

Using the smoothed pressure curves shown in Figure B.3a the speed of sound is computed from equation (B.1). To do so, given the temperature, the pressure and its

Figure B.3: Smoothed curves: (a) $p - v$ plots of smoothed pressure curves at constant temperature (in a logarithmic scale), the magnified view of part of the plots shown at the right side of the figure, and the shifted (liquid) saturation points of the smoothed curves (highlighted line), obtained for $0.005 \leq \rho \leq 1100 \text{ kg m}^{-3}$, and $273.16 \leq T \leq 350 \text{ K}$; (b) $c - \alpha$ (α is vapor void fraction) plots of the acoustic speed of sound curve obtained using the smoothed pressure curves in (a), and the Wallis speed of sound curve, with $T = 298 \text{ K}$.

gradients need to be interpolated from the pressure curves in Figure B.3a. Note that the equation (B.1) contains the gradients of the pressure with respect to ρ and also e . Therefore, the pressure curves need to be smooth in both the $p - \rho$ (or $p - v$) and $p - e$ spaces. Although, the smoothing of the pressure curves in Figure B.3a is carried out only in the $p - v$ ($v = 1/\rho$) space, it was observed that these smoothed pressure curves are also smooth enough in the $p - e$ space. The acoustic speed of sound plots obtained from equation (B.1), with p interpolated from the smoothed pressure curves in Figure B.3a, and for a constant temperature of $T = 298 \text{ K}$ are presented in Figure B.3b. It is observed that the acoustic speed of sound curve is smoothed in the liquid phase region, and on the mixture side (not clearly visible from this figure). Although, the quality of the smoothness of the speed of sound curves is not so good in these figures, it was found out that further smoothing of the curves is not so straightforward. In Figure B.4 the plots of the smoothed pressure and speed of sound curves using different smoothing settings are presented. It is observed that when the pressure curves are over-smoothed, although the speed of sound curves become more smooth, the liquid saturation pressure points in $p - v$ diagram in Figure B.4a are shifted to rather high values. This means that the cavitation trigger takes place at very high pressures, compared to the previously smoothed curves in Figure B.3, which is highly undesirable.

Additionally, other smoothing settings and also different smoothing procedures were tested, which were not satisfactory. It is noticed that, due to very steep gradients of the pressure and speed of sound and also because of the restrictions that must be satisfied to correctly model the physical phenomenon in cavitation, it is not so straightforward to obtain nicely smoothed curves which also satisfy these conditions. However, one can still use these smoothed curves in spite of some modeling errors. Furthermore, alternative smoothing functions can be tested to achieve better smoothed curves. The smoothing approach presented in this chapter, is not utilized in numerical simulations

Figure B.4: Over-smoothened curves: (a) $p - v$ plots of smoothed constant temperature curves for pressure (in a logarithmic scale), the magnified view of part of the plots shown on the right side of the figure, and the shifted (liquid) saturation points of the smoothed curves (highlighted line), with $0.005 \leq \rho \leq 1100 \text{ kg m}^{-3}$, and $273.16 \leq T \leq 350 \text{ K}$; (b) $c - \alpha$ plots of acoustic speed of sound curve obtained using the smoothed pressure curves in (a), and the Wallis speed of sound curve, with $T = 298 \text{ K}$.

presented in this thesis.

Appendix C

GRADIENTS OF THE THERMODYNAMIC RELATIONS

The gradients of the thermodynamic relations in section 2.4.2 are presented in this appendix. The derivation of the gradients is based on the independent variables density and internal energy, i.e. (ρ, e) .

Saturation

Using the definitions of the saturated liquid and vapor densities, i.e. $\rho_{l,sat}$ and $\rho_{v,sat}$, respectively, and the saturated pressure p_{sat} in section 2.4.2, we have:

$$\frac{d\rho_{l,sat}(T)}{dT} = -\frac{\rho_c}{T_c} \sum_{i=1}^7 b_i \hat{b}_i \theta^{\hat{b}_i-1}, \quad (C.1)$$

$$\frac{d\rho_{v,sat}(T)}{dT} = -\frac{\rho_{v,sat}(T)}{T_c} \sum_{i=1}^7 c_i \hat{c}_i \theta^{\hat{c}_i-1}, \quad (C.2)$$

$$\frac{dp_{sat}(T)}{dT} = -p_{sat} \left(\frac{T_c}{T^2} \sum_{i=1}^7 a_i \theta^{\hat{a}_i} + \frac{1}{T} \sum_{i=1}^7 a_i \hat{a}_i \theta^{\hat{a}_i-1} \right). \quad (C.3)$$

Here, T is temperature, $\theta = 1 - T/T_c$, and $a_i, \hat{a}_i, b_i, \hat{b}_i, c_i, \hat{c}_i$ are the constants given in Table 2.1 (taken from Schmidt [10]). These relations are valid for the ranges of temperature with lower and upper limits T_r and T_c , respectively, which are the triple point and the critical point temperatures of water, respectively. The values of the remaining constants are given at the end of this appendix.

Liquid

The thermodynamic expression for pressure p in liquid phase is given in equation (2.13). Using this expression, the gradients of the liquid pressure can be written as follows

$$\left(\frac{\partial p}{\partial e} \right)_\rho = \frac{1}{C_{vl}} \left(-\frac{K_0 N \frac{d\rho_{l,sat}}{dT}(T)}{\rho_{l,sat}(T)} \left(\frac{\rho}{\rho_{l,sat}(T)} \right)^N + \frac{dp_{sat}}{dT}(T) \right), \quad (C.4)$$

$$\left(\frac{\partial p}{\partial \rho} \right)_e = \frac{K_0 N}{\rho} \left(\frac{\rho}{\rho_{l,sat}(T)} \right)^N, \quad (C.5)$$

where, T is temperature, $\rho_{l,sat}$ and p_{sat} are saturated liquid density and saturated pressure, respectively (with expressions given in section 2.4.2), $K_0 = 3.3 \times 10^8$ Pa, and $N = 7.15$ for water, and the values of the other constants can be found at the end of this appendix.

Vapor

Using the expression for pressure p in vapor phase (equation (2.22)), the corresponding gradients can be written as

$$\left(\frac{\partial p}{\partial e}\right)_\rho = \frac{\rho R}{C_{vv}}, \quad (\text{C.6})$$

$$\left(\frac{\partial p}{\partial \rho}\right)_e = RT, \quad (\text{C.7})$$

where, T is temperature. The values of the constants in these relations are given at the end of this appendix.

Mixture

The mixture pressure p is defined in equation (2.37). The mixture pressure gradients are

given by

$$\begin{aligned}
\left(\frac{\partial p}{\partial e}\right)_\rho = & \left(\left(\frac{d}{dT} p_{sat}(T) \right) \rho \left((\rho_{l,sat}(T))^2 - 2 \rho_{l,sat}(T) \rho_{v,sat}(T) + (\rho_{v,sat}(T))^2 \right) \right) \\
& / \left(- C_{vl} \rho \rho_{l,sat}(T) \rho_{v,sat}(T) - C_{vv} \rho \rho_{l,sat}(T) \rho_{v,sat}(T) - L_v (\rho_{v,sat}(T))^2 \right. \\
& \frac{d}{dT} \rho_{l,sat}(T) + L_v (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) - C_{vv} \rho T \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) \\
& + C_{vv} \rho T \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) - C_{vl} T_0 \rho \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) \\
& + C_{vl} T_0 \rho \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) + C_{vl} \rho T \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) \\
& - C_{vl} \rho T \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) + C_{vv} T_0 \rho \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) \\
& - C_{vv} T_0 \rho \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) + C_{vl} T (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) \\
& - C_{vv} T_0 (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) + C_{vv} T_0 (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) \\
& + C_{vv} T (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) - C_{vv} T (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) \\
& - L_v \rho \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) + L_v \rho \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) \\
& + C_{vl} T_0 (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) - C_{vl} T_0 (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) \\
& - C_{vl} T (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) + C_{vv} (\rho_{l,sat}(T))^2 \rho_{v,sat}(T) \\
& + C_{vl} \rho (\rho_{l,sat}(T))^2 + C_{vv} \rho (\rho_{v,sat}(T))^2 - C_{vl} (\rho_{l,sat}(T))^2 \rho_{v,sat}(T) \\
& \left. + C_{vl} \rho_{l,sat}(T) (\rho_{v,sat}(T))^2 - C_{vv} \rho_{l,sat}(T) (\rho_{v,sat}(T))^2 \right), \tag{C.8}
\end{aligned}$$

$$\begin{aligned}
\left(\frac{\partial p}{\partial \rho}\right)_e = & \left(\left(\frac{d}{dT} p_{sat}(T) \right) \rho_{l,sat}(T) \rho_{v,sat}(T) (T \rho_{l,sat}(T) C_{vv} - T \rho_{l,sat}(T) \right. \\
& C_{vl} - T \rho_{v,sat}(T) C_{vv} + T \rho_{v,sat}(T) C_{vl} - \rho_{l,sat}(T) T_0 C_{vv} + \rho_{l,sat} \\
& (T) T_0 C_{vl} + \rho_{v,sat}(T) T_0 C_{vv} - \rho_{v,sat}(T) T_0 C_{vl} + \rho_{l,sat}(T) \\
& L_v - \rho_{v,sat}(T) L_v) \Bigg) \Bigg/ \left(\rho (-C_{vl} \rho \rho_{l,sat}(T) \rho_{v,sat}(T) - C_{vv} \rho \rho_{l,sat}(T) \right. \\
& \rho_{v,sat}(T) - L_v (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) + L_v (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) \\
& - C_{vv} \rho T \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) + C_{vv} \rho T \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) \\
& - C_{vl} T_0 \rho \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) + C_{vl} T_0 \rho \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) \\
& + C_{vl} \rho T \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) - C_{vl} \rho T \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) \\
& + C_{vv} T_0 \rho \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) - C_{vv} T_0 \rho \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) \\
& + C_{vl} T (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) - C_{vv} T_0 (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) \\
& + C_{vv} T_0 (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) + C_{vv} T (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) \\
& - C_{vv} T (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) - L_v \rho \rho_{l,sat}(T) \frac{d}{dT} \rho_{v,sat}(T) \\
& + L_v \rho \rho_{v,sat}(T) \frac{d}{dT} \rho_{l,sat}(T) + C_{vl} T_0 (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) \\
& - C_{vl} T_0 (\rho_{v,sat}(T))^2 \frac{d}{dT} \rho_{l,sat}(T) - C_{vl} T (\rho_{l,sat}(T))^2 \frac{d}{dT} \rho_{v,sat}(T) \\
& + C_{vv} (\rho_{l,sat}(T))^2 \rho_{v,sat}(T) + C_{vl} \rho (\rho_{l,sat}(T))^2 + C_{vv} \rho (\rho_{v,sat}(T))^2 \\
& - C_{vl} (\rho_{l,sat}(T))^2 \rho_{v,sat}(T) + C_{vl} \rho_{l,sat}(T) (\rho_{v,sat}(T))^2 \\
& \left. - C_{vv} \rho_{l,sat}(T) (\rho_{v,sat}(T))^2 \right) \Bigg), \tag{C.9}
\end{aligned}$$

where, T is temperature, $\rho_{l,sat}$ and $\rho_{v,sat}$ are the saturated liquid and vapor densities, respectively, p_{sat} is the saturated pressure. The expressions for the saturated variables and their gradients are given in section 2.4.2, and Appendix C, respectively. Furthermore, the values of the constants in these relations are given below.

The values of the constants used in the preceding expressions for water are: $T_c = 647.16 \text{ K}$, $p_c = 22.12 \times 10^6 \text{ Pa}$, $\rho_c = 322.0 \text{ kg m}^{-3}$ (critical temperature, pressure, and density), $T_r = 273.15 \text{ K}$ (triple point temperature), $C_{vl} = 4180 \text{ J kg}^{-1} \text{ K}^{-1}$ (the liquid specific heat at constant volume), $T_0 = 273.15 \text{ K}$ (a reference temperature), $e_{l0} = 617.0 \text{ J kg}^{-1}$ (a reference internal energy), $L_v(T_0) = 2.3753 \times 10^6 \text{ J kg}^{-1}$ (the latent heat of vaporization), $R = 461.6 \text{ J kg}^{-1} \text{ K}^{-1}$ (the specific gas constant), and $C_{vv} = 1410.8 \text{ J kg}^{-1} \text{ K}^{-1}$ (the specific heat at constant volume).

Appendix $\mathcal{D}$

TRIANGULATION TYPES IN POITC APPROACH

The different types of the triangulations used in the POITC approach are shown in Figure D.1. The data nodes are numbered for each case. The numbering of the nodes is chosen such that the connectivity matrix of the triangular elements (denoted by $\underline{\underline{M}}_{conn}$) in each triangulated transition cell belongs to one of the three types shown in equation (D.1). The first connectivity matrix $\underline{\underline{M}}_{conn}^1$ is defined for the cases (a), (b), (e), (f), (h), and (i), the second one $\underline{\underline{M}}_{conn}^2$ for the cases (c) and (j), and finally the third one $\underline{\underline{M}}_{conn}^3$ for the cases (d), (g), and (k).

$$\underline{\underline{M}}_{conn}^1 = \begin{bmatrix} 2 & 5 & 1 \\ 5 & 6 & 1 \\ 3 & 6 & 5 \\ 4 & 1 & 6 \end{bmatrix}, \quad \underline{\underline{M}}_{conn}^2 = \begin{bmatrix} 2 & 3 & 5 \\ 6 & 5 & 3 \\ 5 & 6 & 1 \\ 4 & 1 & 6 \end{bmatrix}, \quad \underline{\underline{M}}_{conn}^3 = \begin{bmatrix} 3 & 2 & 6 \\ 6 & 2 & 5 \\ 5 & 4 & 6 \\ 1 & 4 & 5 \end{bmatrix} \quad (D.1)$$

Figure D.1: Continued, next page

Figure D.1: The types of triangulations of transition cells in POITC approach, with the cases (a) - (g) for liquid-mixture state, and the cases (h) - (k) for the vapor-mixture state. The saturation line is highlighted in each case.

Appendix $\mathcal{E}$

TRIANGULAR BARYCENTRIC COORDINATES

In this appendix, the properties of the barycentric coordinates in triangular elements are described.

E.1 Determining whether or not a point is inside the triangle

The barycentric coordinates properties are utilized in order to determine whether or not a target point is inside the triangular element. In Figure E.1 a triangular element and its vertices Cartesian coordinates with $\mathbf{v}_1 = (\rho_1, e_1)$, $\mathbf{v}_2 = (\rho_2, e_2)$, $\mathbf{v}_3 = (\rho_3, e_3)$ are presented. In the same figure, the coordinates of a target point with $\hat{\mathbf{v}} = (\hat{\rho}, \hat{e})$ are also shown. The coordinates of $\hat{\mathbf{v}}$ can be written in terms of the components of the triangle vertices coordinates $\mathbf{v}_i$ as follows

$$\hat{\mathbf{v}} = \hat{\lambda}_i \mathbf{v}_i, \quad i = \{1, \dots, 3\}. \quad (\text{E.1})$$

Here, $\hat{\lambda}_i = \{\hat{\lambda}_1, \hat{\lambda}_2, \hat{\lambda}_3\}$ are the barycentric coefficients which need to be computed. For the computed $\hat{\lambda}_i$, if $0 \leq \hat{\lambda}_i \leq 1$ for all $i = \{1, \dots, 3\}$, then the point is inside or on the sides of the triangle. Otherwise, the point is outside the triangle. For the barycentric coefficients we have $\hat{\lambda}_1 + \hat{\lambda}_2 + \hat{\lambda}_3 = 1$, which gives $\hat{\lambda}_3 = 1 - \hat{\lambda}_1 - \hat{\lambda}_2$. With this condition the unknowns are reduced to $\{\hat{\lambda}_1, \hat{\lambda}_2\}$.

Equation E.1 in component form can be written as follows

$$\hat{\rho} = \hat{\lambda}_1 \rho_1 + \hat{\lambda}_2 \rho_2 + (1 - \hat{\lambda}_1 - \hat{\lambda}_2) \rho_3, \quad (\text{E.2})$$

$$\hat{e} = \hat{\lambda}_1 e_1 + \hat{\lambda}_2 e_2 + (1 - \hat{\lambda}_1 - \hat{\lambda}_2) e_3, \quad (\text{E.3})$$

or

$$\hat{\lambda}_1 (\rho_1 - \rho_3) + \hat{\lambda}_2 (\rho_2 - \rho_3) = \hat{\rho} - \rho_3, \quad (\text{E.4})$$

$$\hat{\lambda}_1 (e_1 - e_3) + \hat{\lambda}_2 (e_2 - e_3) = \hat{e} - e_3. \quad (\text{E.5})$$

Equations (E.4) and (E.5) can be rewritten in a matrix form as

$$\underline{\hat{T}} \cdot \underline{\hat{\lambda}} = \hat{\mathbf{v}} - \mathbf{v}_3, \quad (\text{E.6})$$

Figure E.1: Schematic of a triangular element showing the coordinates of the vertices of the triangle and a target point inside the triangle.

where, $\hat{\lambda}$ and $\underline{\hat{T}}$ are the vector of the barycentric coefficients and a transformation matrix, respectively, given by

$$\hat{\lambda} = \begin{pmatrix} \hat{\lambda}_1 \\ \hat{\lambda}_2 \end{pmatrix}, \quad \underline{\hat{T}} = \begin{pmatrix} \rho_{31} & \rho_{32} \\ e_{31} & e_{32} \end{pmatrix}. \quad (\text{E.7})$$

Here, the components of $\underline{\hat{T}}$ are in difference form, which are written by using the following definition with $\psi_{lm} = \psi_m - \psi_l$ for a variable ψ .

The $\hat{\lambda}_1$ and $\hat{\lambda}_2$ coefficients are derived from equation (E.6) as follows

$$\begin{pmatrix} \hat{\lambda}_1 \\ \hat{\lambda}_2 \end{pmatrix} = \underline{\hat{T}}^{-1} (\hat{\mathbf{v}} - \mathbf{v}_3). \quad (\text{E.8})$$

Note that $\underline{\hat{T}}$ is an invertible matrix. This is because the columns of $\underline{\hat{T}}$ are the side vectors of the triangle which are linearly independent (otherwise these vectors would not form a triangle). Therefore, as long as the triangles are formed correctly, the determinant of $\underline{\hat{T}}$, i.e. $|\underline{\hat{T}}|$, never becomes zero, which shows that the $\underline{\hat{T}}$ matrix is invertible. Finally, the expressions for $\hat{\lambda}_1$ and $\hat{\lambda}_2$ can be written as follows

$$\begin{pmatrix} \hat{\lambda}_1 \\ \hat{\lambda}_2 \end{pmatrix} = \frac{1}{|\underline{\hat{T}}|} \begin{pmatrix} e_{32} (\hat{\rho} - \rho_3) + \rho_{23} (\hat{e} - e_3) \\ e_{13} (\hat{\rho} - \rho_3) + \rho_{31} (\hat{e} - e_3) \end{pmatrix}, \quad (\text{E.9})$$

and $\hat{\lambda}_3$ is computed from the known values of $\hat{\lambda}_1$ and $\hat{\lambda}_2$ as $\hat{\lambda}_3 = 1 - \hat{\lambda}_1 - \hat{\lambda}_2$.

E.2 Interpolation of the variables

Once, using the procedure in the preceding section, it has been determined that the target point is inside the triangle, a variable Ψ at this point can be computed by interpolation also by using the barycentric coordinates properties. Using the known values of the barycentric coefficients $\hat{\lambda}_i$, the variable $\hat{\Psi} \equiv \Psi(\hat{\mathbf{v}})$ at the target point is interpolated using the following barycentric formulation

$$\hat{\Psi} = \hat{\lambda}_i \Psi_i, \quad \{i = 1, \dots, 3\} \quad (\text{E.10})$$

where, $\Psi_i \equiv \Psi(\mathbf{v}_i)$ denotes the values of the variable Ψ at the vertices i of the triangle. Furthermore, since the point is inside the triangle we have $0 \leq \hat{\lambda}_i \leq 1$ (see section E.1).

Appendix $\mathcal{F}$

THIRD-ORDER ACCURATE WENO COEFFICIENTS ON NON-UNIFORM STRUCTURED GRIDS

In this appendix, the coefficients for a third-order accurate ($m = 2$ in equation (4.73)) WENO scheme on non-uniform structured grids are given. The coefficients are derived for a location x_{k+k_c} , with $-1/2 \leq \frac{x_{k+k_c} - x_k}{\Delta x_k} \leq 1/2$ and $\Delta x_k = x_{k+1/2} - x_{k-1/2}$, inside a cell I_k in a grid stencil $S(k) := \{I_{k-r}, \dots, I_{k-r+m-1}\}$ with a left shift $0 \leq r \leq m-1$. In particular this includes the left and right states of the faces $k+1/2$ and $k-1/2$ of the cell I_k , respectively. Moreover, when the stencil $S(k)$ is utilized to reconstruct the variables on both the left and right states of a face $k+1/2$, i.e. $q_{k+1/2}^\mp$, extra coefficients considering an additional left shift with $r = -1$ in the stencil are also provided.

F.1 Polynomial coefficients

From equation (4.79), the polynomial coefficients c_{rj} for a point x_{k+k_c} inside the cell I_k with $0 \leq r \leq m-1$ and $0 \leq j \leq m-1$ are given by

$$\begin{aligned} c_{00} &= \frac{2x_{k+k_c} - x_{k+3/2} - x_{k-1/2}}{x_{k+1/2} - x_{k+3/2}} + \frac{(2x_{k+k_c} - x_{k+1/2} - x_{k-1/2})(x_{k+1/2} - x_{k-1/2})}{(x_{k+3/2} - x_{k-1/2})(x_{k+3/2} - x_{k+1/2})}, \\ c_{01} &= \frac{2x_{k+k_c} - x_{k+1/2} - x_{k-1/2}}{x_{k+3/2} - x_{k-1/2}}, \end{aligned} \quad (\text{F.1})$$

$$\begin{aligned} c_{10} &= \frac{2x_{k+k_c} - x_{k+1/2} - x_{k-3/2}}{x_{k-1/2} - x_{k+1/2}} + \frac{(2x_{k+k_c} - x_{k-1/2} - x_{k-3/2})(x_{k-1/2} - x_{k-3/2})}{(x_{k+1/2} - x_{k-3/2})(x_{k+1/2} - x_{k-1/2})}, \\ c_{11} &= \frac{2x_{k+k_c} - x_{k-1/2} - x_{k-3/2}}{x_{k+1/2} - x_{k-3/2}}, \end{aligned} \quad (\text{F.2})$$

which can also be used for the reconstruction of the cell I_k faces, i.e. the left state of the face $k+1/2$ at $x_{k+k_c} = x_{k+1/2}$ and the right state of the face $k-1/2$ at $x_{k+k_c} = x_{k-1/2}$. When the reconstruction is performed on both the left and right states of a face $k+1/2$ using the same stencil $S(k)$, for the right state of the face inside the cell $k+1$ with $x_{k+1+k_c} = x_{k+1/2}$ an additional left shift with $r = -1$ is also considered in the stencil, and the simplified expressions for the corresponding c_{rj} coefficients are

given by

$$\begin{aligned} c_{-10} &= \frac{(x_{k+3/2} - x_{k+1/2}) + (x_{k+5/2} - x_{k+1/2})}{x_{k+5/2} - x_{k+1/2}}, \\ c_{-11} &= -\frac{x_{k+3/2} - x_{k+1/2}}{x_{k+5/2} - x_{k+1/2}}. \end{aligned} \quad (\text{F.3})$$

F.2 Ideal weights

The ideal weights d_r with $0 \leq r \leq m-1$ for a point x_{k+k_c} inside the cell I_k are given by

$$\begin{aligned} d_0 &= \frac{(x_{k-1/2} - x_{k+k_c})(x_{k+1/2} - 2x_{k+k_c} + x_{k-3/2})}{(-x_{k+3/2} + x_{k-3/2})(x_{k-1/2} + x_{k+1/2} - 2x_{k+k_c})} \\ &\quad - \frac{(x_{k+k_c} - x_{k-3/2})(-x_{k+k_c} + x_{k+1/2})}{(-x_{k+3/2} + x_{k-3/2})(x_{k-1/2} + x_{k+1/2} - 2x_{k+k_c})}, \end{aligned} \quad (\text{F.4})$$

$$\begin{aligned} d_1 &= \frac{(x_{k+3/2} - x_{k+k_c})(x_{k-1/2} + x_{k+1/2} - 2x_{k+k_c})}{(-x_{k+3/2} + x_{k-3/2})(x_{k-1/2} + x_{k+1/2} - 2x_{k+k_c})} \\ &\quad + \frac{(x_{k-1/2} - x_{k+k_c})(-x_{k+k_c} + x_{k+1/2})}{(-x_{k+3/2} + x_{k-3/2})(x_{k-1/2} + x_{k+1/2} - 2x_{k+k_c})}, \end{aligned} \quad (\text{F.5})$$

which can also be used for the reconstruction of the cell I_k faces, i.e. the left state of the face $k+1/2$ at $x_{k+k_c} = x_{k+1/2}$ and the right of state of the face $k-1/2$ at $x_{k+k_c} = x_{k-1/2}$. When the reconstruction is performed on both the left and right states of a face $k+1/2$ using the same stencil $S(k)$, for the right state of the face inside the cell $k+1$ with $x_{k+1+k_c} = x_{k+1/2}$ an additional left shift with $r = -1$ is also needed. The simplified expressions for d_r coefficient with $r = -1$ is given by

$$d_{-1} = \frac{x_{k+1/2} - x_{k-1/2}}{x_{k+5/2} - x_{k-1/2}}. \quad (\text{F.6})$$

F.3 Smoothness indicator coefficients

The smoothness indicator coefficients β_r with $0 \leq r \leq m-1$ for the cell I_k are given by:

$$\beta_0 = \left(\frac{4\Delta x_k^2}{(x_{k+3/2} - x_{k-1/2})^2} \right) (v_{k+1} - v_k)^2, \quad (\text{F.7})$$

$$\beta_1 = \left(\frac{4\Delta x_k^2}{(x_{k+1/2} - x_{k-3/2})^2} \right) (v_k - v_{k-1})^2, \quad (\text{F.8})$$

which can also be used for the reconstruction of the variables on the cell I_k faces. When the reconstruction is performed on both the left and right states of a face $k+1/2$ using the same stencil $S(k)$, for the right state of the face inside the cell $k+1$ an additional coefficient with a left shift $r = -1$ is also needed:

$$\beta_{-1} = \left(\frac{4\Delta x_{k+1}^2}{(x_{k+5/2} - x_{k+1/2})^2} \right) (v_{k+2} - v_{k+1})^2. \quad (\text{F.9})$$

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