A multi-component real-fluid two-phase flow solver with high-order finite-difference schemes

Jian-Hang Wang\textsuperscript{1,2,*}, Songzhi Yang\textsuperscript{2,3}, Chaouki Habchi\textsuperscript{2,3}, Xiangyu Y. Hu\textsuperscript{1}, Nikolaus A. Adams\textsuperscript{1}

\textsuperscript{1}Chair of Aerodynamics and Fluid mechanics, Department of Mechanical Engineering, Technical University of Munich, Boltzmannstr. 15, 85748 Garching, Germany
\textsuperscript{2}IFP Energies nouvelles, 1 et 4 avenue de Bois-Préau, 92852 Rueil-Malmaison, France
\textsuperscript{3}Institut Carnot IFPEN Transports Energie, 1 et 4 avenue de Bois-Préau, 92852 Rueil-Malmaison, France

*Corresponding author: jianhang.wang@tum.de

Abstract

In this study, a mass-fraction based fully conservative multi-component two-phase flow solver is considered using characteristic-wise finite-difference (CWFD) discretization with the 5th-order WENO scheme, in order to reduce numerical interface smearing and oscillations. Real-fluid thermodynamic properties are accounted for by a vapor-liquid equilibrium (VLE) model according to the local total density, internal energy and composition of the homogeneous mixture, with each phase being separately described by its Peng-Robinson equation of state (PR-EoS). A multi-component Roe averaging for the cell-face eigen-system in CWFD methods has been developed with pressure derivatives resulted from the VLE model. Several 1D testing examples, e.g. interface advection, shock-tube problems and double-expansion cavitation, have been examined to demonstrate the low-oscillation, low-dissipation and robust performance of the present solver, in comparison with finite-volume schemes. A 2D transcritical injection process has also been simulated. It has been shown that high-order numerical schemes, such as the current CWFD method may be the way to reduce the smearing in diffuse interface modelling.

Keywords

Two-phase flow, phase equilibrium, finite difference method, Roe averaging, transcritical, fuel injection

Introduction

Accurate and robust simulation of compressible real-fluid two-phase flow is crucial for many engineering applications, such as the fuel injection in internal combustion engines. One example is that, in diesel engines when the liquid fuel is injected into the ambient gas at a pressure higher than its critical value, the fuel jet will be heated to supercritical temperature before combustion takes place. This process is often referred to as transcritical injection [1]. Intensive fluid-dynamical structures and thermodynamical processes may happen in the typical complex two-phase flow. Simulation of such complicated unsteady, multi-scale two-phase flows with multiple fluids of thermodynamic properties is very challenging. Accurate flow solver with the capability of capturing high-resolution interface and real-fluid thermodynamic solver which can precisely describe phase and component states under varying temperature and pressure conditions are greatly desired [1, 2, 3].

Regarding the flow solver, diffuse-interface methods are widely used with various numerical schemes. Both fully conservative (FC) schemes [4, 5, 6, 7, 8, 9] and quasi-conservative schemes (QC) [10, 11, 12, 13, 14, 15] have been intensively studied and used for two-phase flow simulation. One advantage of the QC schemes lies in avoiding the occurrence of spurious pressure oscillations [16], at a sacrifice of losing the strict energy conservation. However, most of the above flow solvers consider finite-volume (FV) schemes due to low computational cost, robust performance and body-fitted nature towards complicated configurations, and limited attention has been paid to finite-difference (FD) schemes for real-fluid two-phase flow simulation. In single-fluid flow simulation of gas dynamics or multi-species flow simulation of chemically reacting gas mixtures, FD schemes have been widely used for capturing strong shocks and detonation waves, etc., owing to high-order accuracy and low-oscillation property. On the other hand, a real-fluid thermodynamics solver is used to precisely determine the local phase and component state under a specific set of internal energy/density or temperature/pressure plus the composition of components. The former solver is the so-called UVn-flash [3] and the latter corresponds to TPn-flash [18]. A simple thermodynamical model of mixture Peng-Robinson equation of state (PR-EoS) [12], without considering phase change or phase separation, can also serve this purpose but it may lead to unphysical or ill-defines states, especially in sub-critical two-phase conditions. The thermodynamic model [7], considering vapor-liquid equilibrium (VLE), can firstly detect whether a state of the fluid mixture corresponds to a point within or outside the two-phase state using the TPD stability analysis [17, 3], and then determines the component state in each phase using mixture cubic EoS. However, a thermodynamically consistent description of mixture thermodynamics is computationally expensive [9] and even dominates the overall CPU time of the integrated solver.

As a result, the present study considers applying the high-order characteristic-wise FD schemes to the mass-fraction based fully conservative multi-component formulation, in order to reduce numerical interface smearing and oscillations, without severely increasing the overall computational cost. Following the work of Ping et al. [3], real-fluid...
thermodynamic properties are accounted for by the VLE model with each phase being described by the mixture PR-EoS, such that either single-phase mixture or two-phase mixture in mechanical and thermodynamical equilibrium or phase change can be described in a thermodynamically generalized and consistent manner.

The remainder of this paper has the following structure. The next section introduces firstly the governing equations and its discretization by the characteristic-wise FD scheme, and then the description of thermodynamic model as well as the UVn-flash solver. Section 3 presents several 1D test examples and a 2D transcritical injection simulation. Conclusions and some prospects are drawn in the last section.

**Methodology**

**Characteristic-wise finite-difference scheme for multi-component Euler equations**

For simplicity and without loss of generality, we solve the two-dimensional compressible multi-component Euler equations in a mass-fraction based fully conservation formulation as follows

\[
U_t + F(U)_x + G(U)_y = 0,
\]

where

\[
U = (\rho, \rho u, \rho v, \rho e, p, \rho y_1, \rho y_2, \cdots, \rho y_{N_y-1})^T,
\]

\[
F(U) = (\rho u, \rho u^2 + p, \rho uv, (\rho e + p)u, \rho y_1 u, \rho y_2 u, \cdots, \rho y_{N_y-1} u)^T,
\]

\[
G(U) = (\rho v, \rho uv, \rho v^2 + p, (\rho e + p)v, \rho y_1 v, \rho y_2 v, \cdots, \rho y_{N_y-1} v)^T,
\]

are vectors of the conserved variables, convective flux in the x or y direction, respectively. The specific total energy including the specific internal energy \(e\) is \(e = e + (\psi^2 + \psi^2)/2\). To close the system, an equation of state (EoS) such as the ideal gas EoS for gas mixtures is usually required. In this study, to avoid unstable thermodynamic states, a thermodynamically consistent solver is used to account for both single-phase and two-phase flow and discussed in the following section.

Shock-capturing schemes are usually employed based on either finite volume (FV) or finite difference (FD) formulation for spatial discretization, in which high-order shock-capturing accuracy as well as high computational efficiency are desired. Low-order FV schemes approximate the cell-face flux function by upwind reconstruction using primitive or conserved variables, together with MUSCL interpolation schemes plus slope limiters and achieve generally second-order accuracy. High-order shock-capturing schemes are realized by characteristic-decomposition flux splitting to assemble the half-point convective flux using high-order interpolation schemes in FD approaches. To achieve high-order FD schemes for Eqs. (1) and (2), Jacobian system including the left and right eigen-vectors as well as Roe-averages of pressure derivatives to calculate the speed of sound \(c\) at the cell face needs to be considered; see details in [19]. It should be noted that, in this study, the adjacent two sets of cell-centered pressure derivatives such as \(\partial p/\partial x\) and \(\partial p/\partial c\) are directly obtained by outputs from the thermo-solver, i.e. UVn-flash, as UVn-flash inherently contains calculations of thermodynamics derivatives (see [3] for details). High-order interpolation scheme WENO5 and local Lax-Friedrich splitting [22] are employed here.

**Vapor-liquid equilibrium model using UVn-flash**

Since the conservative governing equations, at a certain time instant, provide directly conserved variables such as density \(\rho\), total energy \(e\), etc., in order to close the system, primitive variables like temperature \(T\) and pressure \(p\) should be obtained through the conserved variables before entering the next time step. A thermodynamic solver is thus needed for translating the local total density \(\rho\), internal energy \(e\) and the overall composition \(z = (z_i), i = 1, \ldots, N_S\) of the homogeneous mixture to equilibrium temperature \(T\); pressure \(p\) and other thermodynamic variables that reflect the state of the homogeneous multi-component two-phase mixture, as shown in Fig. 1, such as the vapor fraction \(\psi\) and component mole fractions \(x\) and \(y\) in the liquid and vapor phase, respectively. This is the so-called isochoric-isoenergetic flash problem. i.e. UVn-flash. The vapor-liquid equilibrium model is assumed with

\[
\begin{align*}
\rho_l &= \rho_v = \rho, \\
T_l &= T_v = T, \\
\mu_{i,v}(T, p, x) &= \mu_{i,l}(T, p, y), \\
\psi U_v + (1 - \psi) U_l &= U^*, \\
\psi V_v + (1 - \psi) V_l &= V^*,
\end{align*}
\]

where subscripts \(l, v\) denote the liquid and vapor phase, respectively, and \(\mu_i\) represents the chemical potential of component \(i\). Note that all the quantities in Eq. (3) are on a molar basis. In either phase \(l\) or \(v\), components are well-mixed filling its volume \(V_l\) or \(V_v\), and the thermodynamic properties of each single-phase mixture are described using the PR-Eos for \(N_c\)-component mixtures with appropriate mixing rules [3]. The last two equations in Eq. (3) conform to energy and mass conservation, and function as the condition of convergence for the iterative UVn-flash. Once the convergence criterion is reached, the equilibrium temperature \(T\) and pressure \(p\) are obtained; see details of the UVn-flash we consider in the present study in [1, 3] and other relevant solvers, e.g. in [20].

This work is licensed under a Creative Commons 4.0 International License (CC BY-NC-ND 4.0).
One critical difficulty of the present UVn-flash (which is based on the deterministic gradient-dependent quasi-Newton algorithm) lies in the convergence of iterative root-finding for equilibrium $T$ and $\rho$ due to the complex non-linearity of PR-EoS and VLE constraints. Non-convergence might arise especially when the phase boundary is crossed. Therefore, a non-linear global optimization technique with non-deterministic strategies is desired and we can refer to the very popular particle swarm optimization (PSO) algorithm [21], which is a gradients-free metaheuristic algorithm exploiting swarming behavior of organisms to search for optimal solutions. Since PSO is population-based and time-consuming, it is activated only when the conventional UVn-flash fails in converging the equilibrium state.

Results and discussion

In this section, we first present several 1D numerical tests of two-component two-phase flows, to demonstrate the reliability of the proposed CWFD framework. In comparison to the 5th-order CWFD WENO5-LLF scheme, AUSM+ scheme [23] with or without minmod slope limiter (AUSM+/minmod) in the FV formulation is also adopted. Computational timestep which is usually controlled by CFL number for compressible flows is sometimes limited to be much smaller such that UVn-flash manages to handle phase boundaries and drastic jumps of thermodynamic states at adjacent cells and time instants. A 2D transcritical injection of liquid n-dodecane into a chamber of gaseous n-dodecane follows to examine the spatial resolution of typical structures, such as vortices, shear-layer instability and interface, etc, by the high-order CWFD scheme.

1D advection case (Gaussian profile)

The first 1D test case we consider is the transitional advection of n-dodecane ($\text{C}_{12}\text{H}_{26}$)/nitrogen ($\text{N}_2$) mixture at constant pressure of 1 bar and velocity of 100 m/s. The 1D domain is 1 m long and both ends are imposed of the scheme and 1st-order AUSM+ with no slope limiter.

The 1D advection case (Gaussian profile) is

\[
T(x) = T_0 - \frac{\Gamma}{2\pi \beta} \exp \left( -\frac{r^2}{\epsilon} \right),
\]

\[
y_1(x) = y_{1,0} - 0.01 \frac{\Gamma}{2\pi \beta} \exp \left( -\frac{r^2}{\epsilon} \right),
\]

\[
y_2 = 1 - y_1,
\]

where $T_0 = 300$ K, $y_{1,0} = 0.99$ and $r^2 = (x - 0.5)^2$ with $\Gamma = 10$, $\beta = 0.01$ and $\epsilon = 0.02$. We use varying grid resolutions with 25, 50, 100, 125 cells in the domain, respectively, and compute the mixture advection for a complete period till $t = 0.01$ s. $L_1$ norms of errors of density and mass fraction $y_1$ are shown in Fig. 2 and the expected high-order accuracy of the present CWFD scheme is demonstrated, compared to the 2nd-order AUSM+/minmod scheme and 1st-order AUSM+ with no slope limiter.
1D advection case
It is well-known that upwind shock-capturing schemes would gradually smear out the sharp interface during advection due to numerical dissipation, and spurious numerical oscillations of pressure and velocity can be induced by the fully conservative formulation versus the quasi-conservative methods. The present study is not aimed at proposing a cure to alleviate spurious oscillations in the fully conservative formulation but examining the possibility of improving interface resolution as well as reducing spurious oscillations by CWFD schemes in comparison with FV schemes based on cell-face flux reconstruction from primitive variables. The present 1D advection case considers the same setup with the above advection case except that initial temperature and mass fractions exhibit sharp interfaces in the present domain of 1000 grid cells. As shown in Fig. 3, it can be seen that after one complete period of advection, the 5th-order CWFD scheme preserves the very sharp interface compared to the reference solution, apparently better than the 2nd-order AUSM+/minmod scheme result and its 1st-order counterpart. Besides, numerical oscillation of pressure, in this case, of the CWFD scheme is less severe than the 2nd-order FV schemes. This is also the case when high-order FV schemes are utilized in single-fluid flow simulations. However, the 1st-order FV scheme outperforms other two schemes, which is possibly because its numerical dissipation is sufficiently large to suppress the oscillation to occur. In this sense, the 5th-order CWFD scheme is the optimal choice weighing both high interface resolution and low oscillation of pressure.

![Image of Figure 3](image)

**Figure 3.** 1D advection of N\textsubscript{2}/C\textsubscript{12}H\textsubscript{26} mixture. Black solid line: reference solution; red circle line: CWFD WENO5-LLF; purple cross line: FV AUSM\textsuperscript{+}; green square line: FV AUSM\textsuperscript{+}/minmod.

1D shocktube case A
This 1D shocktube case ([24], Fig. 4) considers a 1 m long tube of H\textsubscript{2}O/N\textsubscript{2} mixture with initial condition as

\[ (p, T) = \begin{cases} 
(2 \text{ bar}, 353.79 \text{ K}), & \text{if } x < 0.5 \text{ m}, \\
(1 \text{ bar}, 337.41 \text{ K}), & \text{otherwise},
\end{cases} \]  

with \(y\textsubscript{N\textsubscript{2}} = 0.7\) and \(y\textsubscript{H\textsubscript{2}O} = 0.3\) along the tube. Computation runs until \(t = 1 \text{ ms}\). In Fig. 4, we can see that all the three solutions predict the similar profiles of variables, in which the proposed CWFD WENO5-LLF scheme yields the sharpest shock especially in the velocity profile. The 2nd-order AUSM\textsuperscript{+}/minmod scheme yields very close results as the high-order scheme while the 1st-order AUSM\textsuperscript{+} scheme exhibits much smeared profiles in this shocktube example.

1D shocktube case B
In this shocktube case, we enhance the initial pressure to be similar with Spray A condition with the initial mass fractions of N\textsubscript{2}/n-dodecane are 0.1/0.9, respectively. The initial temperature is 900 K in the left half and 363 K in the right half of the tube, respectively. Computation runs until \(t = 0.3 \text{ ms}\). In Fig. 5, we can see that the CWFD WENO5-LLF scheme and 2nd-order AUSM\textsuperscript{+}/minmod scheme both yield sharp discontinuities. However, the 2nd-order FV scheme also produces more severe numerical oscillations in pressure and velocity profiles. The corresponding 1st-order result is smooth with less accuracy.

1D double-expansion cavitation
The double-expansion case (see the similar double-expansion test in Fig. 7 of [24]) considers the cavitation phenomenon when pressure decreases to be below the saturation pressure as the fluid are extruded outwards from the middle of the 1D tube. Initial conditions of pressure, temperature and mass fraction of H\textsubscript{2}O are 1 bar, 293 K and...
0.99995, respectively. Initial velocity of the left half of the H$_2$O/N$_2$ mixture is -1 m/s while the right half is moving oppositely. The 1D domain is discretized with 100 cells. In Fig. 6, it can be seen that the CWFD scheme preserves the sharpness of the expansion wave, as expected. Note that the 1st-order FV scheme yields a velocity jump in the middle point of the tube, while the 2nd-order FV scheme, although it gives the correct stationary area of $u = 0$, results in a spurious velocity oscillation.

2D transcritical n-dodecane injection

Now we focus on the 2D simulation of the low-temperature (363 K) n-dodecane injected into a chamber of n-dodecane of high temperature 900 K at 60 bar. Inlet pressure and velocity are 70 bar and 55 m/s, respectively. N-dodecane are diluted with nitrogen of a mass fraction of 0.01%. Limited by the computing power, the current simulation runs on a 2D domain of the size $50h \times 8h$, where $h = 100 \mu m$ is the inlet height, as shown in Fig. 7. Two sets of non-uniform grids, both with stretching mesh sizes away from the inlet, are used to save CPU time. Similar simulation has been studied in [1, 25, 26].

In Fig. 8, we display the early evolution of the jet flow at three time instants, using the 5th-order CWFD scheme and 2nd-order FV scheme on two grids, respectively. Referring to the qualitative illustration of liquid jet flow from the DNS results in [25], it is clear to see, from the CWFD results in the first column, the roll-up of a mushroom-like primary vortex followed by several secondary vortices induced along the interface between the primary vortex and the ambient chamber fluid. Rayleigh-Taylor shear-layer instability at the interface bewteen the jet column and the ambient high-temperature fluid induces a series of tiny vortices as well. The CWFD scheme on the coarse grid provides a lower-resolution display of the structures while it preserves similar aforementioned characteristics as in the fine grid. The FV scheme, however, can merely give the symmetric primary vortex structure due to severe numerical viscosity, and it predicts different lengths of the jet from the inlet, based on two grids. The primary vortex
size and location of the FV scheme on the fine grid is similar with the two CWFD results while the coarse FV result has a primary vortex of flatter shape and sharper tip in the front. In Fig. 9, we further discuss the subsequent evolution of the jet flow. More obviously, in the CWFD results on the fine grid, shedding of the secondary vortices from the primary vortex is observed and it either merges with the mainstream of jet column or splashes away into the surrounding fluid. As time goes by, when the jet column cannot preserve its horizontal and straight sharp (marked by B) due to instability and the primary vortex core has a very thin connection with the vortex edges (marked by A), the primary vortex almost breaks up. Despite of the complex flowfield with many unsteady structures, the high-order CWFD scheme can preserve the basic structure of the jet and primary vortex on two grids, especially the similar jet length and size. However, the 2nd-order FV scheme can only capture the stable growth and propagation of the primary vortex, associated with the growing jet column, on either fine or coarse grid. In addition, the smearing of the primary vortex is increasingly severe because of the stretched grid effect when its distance from the inlet increases and the tip of the jet on coarse grid is moving too fast.

It is reasonable to believe that with a high-order spatial scheme on a fine grid, some detailed characteristics of the fundamental flow structures can be numerically captured and it will be interesting to examine if these plentiful structures (which are not available in low-order scheme results) such as vortex shedding, breakup and shear-layer vortices, etc, have a significant effect upon the prediction of realistic injection processes with a larger domain and longer simulation time. Analogically, realistic injection processes usually have plentiful contents of fluid-dynamic and thermodynamic phenomena, such as ligament and droplet formation, atomization, evaporation and spray breakup, etc.

Conclusion

In this study, a multi-component two-phase flow solver utilizing high-order CWFD schemes for the mass-fraction based fully conservative formulation has been presented, in association with the thermodynamic solver UVn-flash based on the VLE model. Both 1D test cases of advection, shocktube and double-expansion problems, and a 2D transcritical injection process demonstrate the considerably high resolution of the present scheme in capturing interfaces, discontinuities and many detailed flow structures of interest. In the future work, it is very interesting to extend the present solver to more realistic industry-level two-phase flow situations like Spray A. Towards a more efficient thermodynamic solver of UVn-flash, a pre-processed tabulation for thermodynamic relations is also desired.

Acknowledgements

The financial support from the EU Marie Sklodowska-Curie Innovative Training Networks (ITN-ETN) (Project ID: 675528-IPPAD-H2020-MSCA-ITN-2015) for the first two authors are gratefully acknowledged. The first author also acknowledge the support for part of this work during his secondment at IFPEN.

This work is licensed under a Creative Commons 4.0 International License (CC BY-NC-ND 4.0).
Figure 8. Density of the 2D transcritical injection. From left to right are CWFD WENO5-LLF on fine grid, AUSM+/minmod on fine grid, CWFD WENO5-LLF on coarse grid and AUSM+/minmod on coarse grid, respectively. From top to bottom are time instants at $t = 5, 10$ and $20 \mu s$, respectively.

References


This work is licensed under a Creative Commons 4.0 International License (CC BY-NC-ND 4.0).
Figure 9. Density of the 2D transcritical injection. Every $2 \times 2$ array of figures are CWFD WENO5-LLF on fine grid, AUSM+/minmod on fine grid, CWFD WENO5-LLF on coarse grid and AUSM+/minmod on coarse grid, respectively. From top to bottom are time instants at $t = 30, 40$ and $50 \mu s$, respectively.