An entropy-stable hybrid scheme for simulations of transcritical real-fluid flows

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ABSTRACT

A finite-volume method is developed for simulating the mixing of turbulent flows at transcritical conditions. Spurious pressure oscillations associated with fully conservative formulations are addressed by extending a double-flux model to real-fluid equations of state. An entropy-stable formulation that combines high-order non-dissipative and low-order dissipative finite-volume schemes is proposed to preserve the physical realizability of numerical solutions across large density gradients. Convexity conditions and constraints on the application of the cubic state equation to transcritical flows are investigated, and conservation properties relevant to the double-flux model are examined. The resulting method is applied to a series of test cases to demonstrate the capability in simulations of problems that are relevant for multi-species transcritical real-fluid flows.

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1. Introduction

The accurate and robust simulation of transcritical real-fluid effects is crucial for many engineering applications, such as fuel injection in internal-combustion engines, rocket motors and gas turbines. For example, in diesel engines, the liquid fuel is injected into the ambient gas at a pressure that exceeds its critical value, and the fuel jet will be heated to a supercritical temperature before combustion takes place. This process is often referred to as a transcritical injection (see Fig. 1). The largest thermodynamic gradient in the transcritical regime occurs as the fluid undergoes a liquid-like to a gas-like transition when crossing the pseudo-boiling line [1], which is shown by the black dashed line in Fig. 1. At elevated pressures, the mixture properties exhibit liquid-like densities and gas-like diffusivities, and the surface tension and enthalpy of vaporization approach zero [2]. This phenomenon was shown by recent experimental studies [1,3,4]. However, these complex processes are still not well understood experimentally and numerically. Therefore, to provide insights into high-pressure combustion systems, reliable numerical simulation tools are required for the characterization of supercritical and transcritical flows.

Due to the unique thermodynamic behavior and large gradients of thermodynamic quantities in the transcritical regime, several challenges must be overcome to enable the numerical prediction of transcritical flows. One challenge is the accurate description of thermodynamic and transport properties across the transcritical regime. Cubic equations of state (EoSs), such as Peng–Robinson (PR) EoS [5] and Soave–Redlich–Kwong (SRK) EoS [6], have been used extensively in transcritical and supercritical simulations for their acceptable accuracy and computational efficiency. Volume-translation methods for cubic EoS were applied to supercritical simulations to further improve the accuracy of thermodynamic descriptions [7]. More complex state equations are also available, such as the Benedict–Webb–Rubin (BWR) EoS [8], and state relations that are
explicit in Helmholtz energy [9], but they often involve complicated implementation and high computational cost. Tabulation methods have been developed and applied to single-species simulations [10]; however, these approaches are generally not extendable to mixtures of more than two species due to the prohibitive memory usage.

Another obstacle in studying transcritical flows with variable thermodynamic properties is the generation of spurious pressure oscillations when a fully conservative scheme is adopted. This is similar to that of multicomponent compressible ideal gas flow calculations [11]. Due to strong nonlinearities of the thermodynamic system, this issue is more severe in transcritical real-fluid flow predictions. The problem cannot be mitigated by introducing numerical dissipation from using lower-order schemes or artificial viscosity, as pointed out in previous works [10,12–15]. Terashima and Koshi [13] solved a transport equation for pressure instead of the total energy equation in their finite-difference solver. This approach was inspired by the work of Karni [16] on multi-species calorically perfect gas, by which the pressure equilibrium can be maintained since pressure is explicitly solved for instead of derived from flow variables. However, for finite-volume schemes, it is not straightforward to solve the pressure equation since pressure is not a conserved quantity. Schmitt et al. [12] derived a quasi-conservative scheme by relating the artificial dissipation terms in the mass, momentum, and energy conservation equations and setting the pressure differential to zero. This procedure was later adopted by Ruiz [14]. The performance of this method to maintain pressure equilibrium across contact discontinuities was not reported. For calorically perfect gas flows, Johnson and Ham [17] adopted a scheme in which an auxiliary advection equation for the specific heat ratio was solved. Although this method is suitable for well-defined interfacial flows with inert species, it is not applicable for thermodynamically complex transcritical and reacting flows in which the thermodynamic properties are dependent on temperature and species compositions. Saurel and Abgrall [18] and Saurel et al. [19,20] developed several methods for interfacial flows where the two phases are solved separately. Recently, Pantano et al. [21] formulated a numerical scheme for transcritical contact and shock problems, which introduced an additive non-conservative transport equation to maintain the mechanical equilibrium of pressure. Another approach originally developed for calorically perfect gas is the double-flux model. This method was proposed by Abgrall and Karni [11], extended by Billet and Abgrall [22] for reacting flows, and later formulated for high-order schemes [23–25]. This quasi-conservative method has been reported to correctly predict shock speeds even for very strong shock waves [11]. In the present work, the double-flux method will be modified and extended to transcritical flows for general real-fluid state equations.

Capturing large density gradients that exist between liquid-like and gas-like fluid phases, as well as diffusion effects at the interfaces subject to strong turbulence, is another challenge that requires consideration. A contact interface with a density ratio on the order of O(100) can be obtained in the transcritical regime. One way to address these large density gradients is to introduce artificial viscosity [13,14,26]. Another approach is to consider hybrid schemes, which combine a high-order non-dissipative flux with an upwind-biased flux to minimize numerical dissipation. For ideal gas flows, multiple applications have shown the performance for predicting turbulent flows using hybrid schemes [27–29]. However, the performance of hybrid schemes on transcritical real-fluid flows has not been evaluated. Entropy-stable concepts were shown to be related to the dissipation in numerical schemes [30]. It was shown that entropy-stable schemes can dampen numerical oscillations across the contact interface [31]. For high-order unstructured finite-volume schemes, it is generally not easy to fulfill the entropy-stability condition, and these schemes have so far not been applied to transcritical flows. By addressing this issue, the objective of this work is to develop a numerical method that is capable of simulating transcritical real-fluid turbulent flows robustly, accurately, and efficiently. Specifically, the following aspects will be addressed:

![Fig. 1. Transcitical regime plotted as a function of reduced pressure, $p_r$, and reduced temperature, $T_r$. Iso-contours of the compressibility factor of oxygen are overlaid. The black solid line indicates the liquid–gas coexistence line and the black dashed line illustrates the pseudo-boiling line in the supercritical region.](image-url)
• Analysis of the generation mechanism of spurious pressure oscillations in the context of transcritical flows and the extension of a double-flux approach [11] to real-fluid flows;
• Formulation of a hybrid scheme using an entropy-stable flux to accurately represent large density gradients and to ensure numerical stability in application to turbulent flows;
• Efficient implementation of the numerical schemes for practical applications of transcritical flows.

The remainder of this paper is structured as follows: Section 2 introduces the governing equations, followed by Section 3, providing the description of thermodynamic relations and transport properties related to transcritical fluids. Section 4 discusses spurious pressure oscillations related to the solution of fully conservative formulations, the development of the double-flux method for real-fluid flows, and the entropy-stable hybrid scheme to represent large density gradients in transcritical flows. In Section 5, a series of test cases is considered and results are compared with available data in literature to examine the capability of this scheme for dealing with real-fluid thermodynamics while maintaining robustness and high-order accuracy. The paper finishes with conclusions in Section 6.

2. Governing equations

The governing equations are the conservation of mass, momentum, total energy, and species, which take the following form:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1a}
\]

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) = \nabla \cdot \mathbf{\tau}, \tag{1b}
\]

\[
\frac{\partial (\rho e_t)}{\partial t} + \nabla \cdot ((\rho e_t + p) \mathbf{u}) = \nabla \cdot (\mathbf{\tau} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q}, \tag{1c}
\]

\[
\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = \nabla \cdot (\rho D_k \nabla Y_k), \text{ for } k = 1, \ldots, N_S - 1, \tag{1d}
\]

where \( \rho \) is the density, \( \mathbf{u} = (u, v, w)^T \) is the velocity vector, \( p \) is the pressure, \( e_t \) is the specific total energy, \( Y_k \) is the mass fraction of species \( k \), \( D_k \) is the diffusion coefficient for species \( k \), and \( N_S \) is the number of species. The viscous stress tensor and heat flux are written as:

\[
\mathbf{\tau} = \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I}, \tag{2a}
\]

\[
\mathbf{q} = -\lambda \nabla T - \rho \sum_{k=1}^{N_S} h_k D_k \nabla Y_k, \tag{2b}
\]

where \( T \) is the temperature, \( \mu \) is the dynamic viscosity, \( \lambda \) is the thermal conductivity, and \( h_k \) is the partial enthalpy of species \( k \). The total energy is related to the internal energy and the kinetic energy:

\[
\rho e_t = \rho e + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u}. \tag{3}
\]

The system is closed with a state equation, which is here written in general form as

\[
p = f(\rho, e, Y_k). \tag{4}
\]

The formulation of the state equation will be discussed in detail in the next section.

A finite-volume approach is utilized for the discretization of the system of equations, Eq. (1):

\[
\frac{\partial U}{\partial t} V_{cv} + \sum_f F^e A_f = \sum_f F^v A_f, \tag{5}
\]

where \( U = [\rho, \rho u, \rho v, \rho w, \rho e_t, \rho Y_k]^T \) is the vector of conserved variables, \( F^e \) is the face-normal Euler flux vector, \( F^v \) is the face-normal viscous flux vector which corresponds to the right-hand side (RHS) of Eq. (1), \( V_{cv} \) is the volume of the control volume, and \( A_f \) is the face area. In the following, if the Euler system is solved, viscous effects are not considered, so that the RHS of Eq. (1) is neglected; Otherwise, the viscous flux is discretized in the same way as described in Pecnik et al. [32]. The numerical schemes developed in the present study focus on the hyperbolic part of the system. A Strang-splitting scheme [33] is applied to separate the convection and diffusion operators of the system. A strong stability preserving 3rd-order Runge–Kutta (SSP-RK3) scheme [34] is used for time integration.
3. Thermodynamic relations

3.1. Equation of state

The numerical framework developed in this work is not limited to a single type of EoS. For computational efficiency and the accurate representation of the thermodynamic state near the critical point [35], the PR cubic EoS [5,36] is used in this study. This state equation can be written as:

\[ p = \frac{RT}{v - b} - \frac{a}{v^2 + 2bv - b^2}, \tag{6} \]

where \( R \) is the gas constant, \( v \) is the specific volume, and the coefficients \( a \) and \( b \) are dependent on temperature and composition to account for effects of intermolecular forces. Extended corresponding states principle and pure fluid assumption for mixtures are adopted [37,38]. The mixing rules and the procedures for evaluating thermodynamic quantities using PR-EoS are presented in Appendix A for the completeness of this study.

The numerical schemes developed in this study are designed for conditions with equilibrium thermodynamic states at a supercritical pressure. As such, phenomena involving metastable thermodynamic states or phase separations [19] are beyond the scope of this work. The hyperbolicity of the convection part of the governing equations with a cubic EoS is discussed in detail in Appendix B. Analysis of simulation results shows that all test cases considered in the present work remain in the hyperbolic region of the governing equations with the PR EoS used, as shown in Appendix B.

3.2. Transport properties

The dynamic viscosity and thermal conductivity are evaluated using Chung’s method with high-pressure correction [39,40]. This method is known to produce oscillations in viscosity for multi-species mixtures when both positive and negative acentric factors are present for individual species [15,41]. To solve this problem, a mole-fraction-averaged viscosity that is evaluated from the viscosity of each individual species can be used. In this study, the negative acentric factor is set to zero only when evaluating the viscosity so that the anomalies in the viscosity are removed. It was found through numerical tests that this approach has similar behavior to the mole fraction-averaged approach.

Takahashi’s high-pressure correction [42] is used to evaluate binary diffusion coefficients. Since only binary mixtures are involved in all test cases studied in this work, the binary diffusion coefficient is the only property needed for the species equations and the evaluation of diffusion coefficients is exact. For more complex mixtures, a mixture-averaged or multicomponent treatment of the diffusion coefficient can be adopted [41].

4. Numerical methods

4.1. Spurious pressure oscillations

One major issue that exists in numerical simulations of transcritical flows is the occurrence of spurious pressure oscillations. This is related to nonlinearities introduced by the real-fluids EoS. To understand the cause of these spurious pressure oscillations and its sensitivity in transcritical simulations, in the following, we consider the relation between internal energy and pressure. This analysis extends the pioneering work by Abgrall and Karni [11]. For a general multicomponent fluid, the internal energy is a nonlinear function of the thermodynamic state (e.g. Eq. (39)). From basic thermodynamics, we have

\[ de = Tds - p dv + \sum_{k=1}^{N_S} \mu_k dY_k, \tag{7a} \]

\[ dh = Tds + v dp + \sum_{k=1}^{N_S} \mu_k dY_k, \tag{7b} \]

where \( \mu_k \) is the mass-specific chemical potential of species \( k \). For simplicity, mass fractions are assumed to be fixed in the following analysis so that the contribution from the mass differential is not explicitly considered. Combining Eq. (7) with the following thermodynamic relations [43]

\[ ds = \frac{c_v dT}{T} + \left( \frac{\partial p}{\partial T} \right)_v dv, \tag{8a} \]

\[ ds = \frac{c_p dT}{T} - \left( \frac{\partial v}{\partial T} \right)_p dp, \tag{8b} \]

where \( c_v \) and \( c_p \) are the specific heats at constant volume and constant pressure, respectively. After some algebra we obtain
\[
\begin{align*}
\frac{de}{\gamma - 1} = & \left( \frac{\partial p}{\partial T} \right)_v v dT + \frac{T}{\gamma - 1} \left( \frac{\partial v}{\partial T} \right)_p dp,
\end{align*}
\]  
(9)

where \( \gamma = c_p/c_v \) is the specific heat ratio.

The above equation can be further expressed through the compressibility factor, \( Z \), which is defined as

\[
Z = \frac{p v}{RT},
\]  
(10)

and the partial derivatives are expressed as

\[
\begin{align*}
\left( \frac{\partial p}{\partial T} \right)_v &= \frac{ZR}{T} + \frac{RT}{v} \left( \frac{\partial Z}{\partial T} \right)_v, \\
\left( \frac{\partial v}{\partial T} \right)_p &= \frac{ZR}{p} + \frac{RT}{p} \left( \frac{\partial Z}{\partial T} \right)_p, \\
\left( \frac{\partial p}{\partial v} \right)_T &= \frac{p}{v} + \frac{RT}{v} \left( \frac{\partial Z}{\partial v} \right)_T.
\end{align*}
\]  
(11a-b-c)

Moreover, we define an effective specific heat ratio or a general adiabatic exponent, \( \gamma^* \), by mimicking the expression for the speed of sound for a calorically perfect gas:

\[
\gamma^* = \frac{\rho c^2}{p}.
\]  
(12)

Using Eq. (45) it can be shown that

\[
\gamma^* = \gamma \left[ 1 - \frac{v}{Z} \left( \frac{\partial Z}{\partial v} \right)_T \right].
\]  
(13)

Note that for an ideal gas, \( \gamma \) and \( \gamma^* \) will become identical since the compressibility factor is constant. Note that if a multi-species mixture is considered, \( \gamma \) will be a nonlinear function of mixture composition and may not be constant.

Inserting Eq. (11) and (13) into Eq. (9) and after some rearrangement we have

\[
\frac{de}{\gamma - 1} = \frac{1}{\gamma^* - 1} d(pv) + \frac{\gamma}{\gamma - 1} \frac{T}{Z} \left( \frac{\partial Z}{\partial T} \right)_v p dv + \frac{1}{\gamma - 1} \frac{T}{Z} \left( \frac{\partial Z}{\partial p} \right)_v dp
\]  
(14a)

\[
= \frac{1}{\gamma^* - 1} d(pv) + \frac{-\gamma}{Z} \left( \frac{\partial Z}{\partial T} \right)_T d(pv) + \frac{\gamma}{\gamma - 1} \frac{T}{Z} \left( \frac{\partial Z}{\partial T} \right)_v p dv + \frac{1}{\gamma - 1} \frac{T}{Z} \left( \frac{\partial Z}{\partial p} \right)_v dp.
\]  
(14b)

Note that since for an ideal gas, the compressibility factor \( Z \) is a constant, the last three terms on the RHS of Eq. (14b) vanish. Further, if we consider a calorically perfect gas, meaning constant \( \gamma^* \) or \( \gamma \), then the following relation between internal energy and pressure can be recovered,

\[
e = \frac{pv}{\gamma - 1} + e_0,
\]  
(15)

where \( e_0 \) is the internal energy at a reference temperature, which is typically set to zero in numerical simulations. Without loss of generality, we can write the specific internal energy for a general fluid in the following form,

\[
e = \frac{pv}{\gamma^* - 1} + e_0^*.
\]  
(16)

where \( \gamma^* \) and \( e_0^* \) can be nonlinear functions of the thermodynamic states and may not be constant as for calorically perfect gases.

After having established an equivalent formulation for a general fluid representation, we will next examine the source of pressure fluctuations that arise from nonlinearities and variations of the specific heat ratio and internal energy. For this, we consider Eq. (16) as EoS, and solve the Euler system of Eq. (1) for a contact interface problem where pressure and velocity are constant at time step \( t^n \). Using a first-order Godunov scheme with upwinding flux for one time step, following the analysis of [22], we have

\[
\delta \rho_j = - \frac{\Delta t}{\Delta x} u_j^n \Delta \rho^n,
\]  
(17a)

\[
\delta (\rho u)_j = - \frac{\Delta t}{\Delta x} (u_j^n)^2 \Delta \rho^n,
\]  
(17b)
where $\Delta t$ is the time step size, $\Delta x$ is the grid spacing, $\delta(t) = (t)^{n+1} - (t)^n$ represents the temporal variation, and $\Delta(t) = (t) - (t)_{j-1}$ is the spatial variation. It can be shown that after one time-step, the velocity maintains equilibrium,

$$u_j^{n+1} = u_j^n.$$  \hfill (18)

With Eq. (16) and the total energy equation, the following expression for the change in pressure can be obtained,

$$\rho_j^{n+1} \delta \varepsilon_{0,j} + p_j^n \delta \left( \frac{1}{\gamma_j^{n+1} - 1} \right) + \frac{1}{\gamma_j^{n+1}} - 1 \delta p_j = - \frac{\Delta t}{\Delta x} u_j^n \left[ \rho_j^{n} \Delta \varepsilon_{0,j}^{n} + p_j^n \Delta \left( \frac{1}{\gamma_j^{n+1} - 1} \right) \right].$$ \hfill (19)

It can be seen that as long as $\gamma^*$ and $\varepsilon_0^*$ are not constant, or that the internal energy $\varepsilon$ is not linear in both pressure and density, then pressure oscillations cannot be maintained across the interface. This is true when a fully conservative scheme is used for the Euler system of Eq. (1). From Eq. (19), it can be seen that oscillations in pressure are related to the jump in $1/(\gamma^* - 1)$ and $\varepsilon_0^*$ both in space and in time.

The nonlinearity between the coupling of internal energy, density and pressure could result from different situations:

- One situation is the ideal-gas multi-fluids case where $\gamma^*$ (equal to $\gamma$) will be a nonlinear function of the mass fractions. Since an ideal gas is used, $\varepsilon_0^*$ (equal to $\varepsilon_0$) is constant;
- When $c_p$ and $c_v$ are not constant, which is typical for reacting cases, $\gamma^*$ will also be a nonlinear function of the thermodynamic states even if an ideal-gas EoS is being used. The internal energy will also be a non-linear function of density and pressure;
- When a general EoS is used and compressibility effects are considered, both $\gamma^*$ and $\varepsilon_0^*$ are nonlinearly related to the internal energy.

For transcritical simulations, which typically involve multi-species and chemically reacting flows with a general EoS, it can be seen that all the above situations are present. Figure 2 shows the compressibility factor and the effective specific heat ratio of nitrogen at various pressures between 50 K and 600 K. The nonlinearity from the cubic real-fluid EoS can be clearly seen. With increasing pressure, this nonlinearity is reduced since the difference between liquid and gas when crossing the pseudo-boiling region becomes smaller [1,44,45]. The results for $\gamma^*$ also explain why for transcritical simulations, pressure oscillations are substantially more severe than for conditions involving ideal gases. For example, at all pressures considered, $\gamma^*$ is $O(100)$ when the temperature is below the critical value; however, for gaseous conditions, the specific heat ratio remains $O(1)$. Moreover, across the narrow temperature range of the pseudo-boiling region, $\gamma^*$ changes dramatically, as compared to the slowly increasing behavior in the higher temperature region. From Eq. (19), if we focus on the terms involving the jump in $\gamma^*$ and omit super- and subscripts for simplicity, it can be seen that $\Delta p/p \sim \Delta [1/(\gamma^* - 1)]$. In Fig. 2(b), a jump from almost zero to about two can be observed for $1/(\gamma^* - 1)$ across the pseudo-boiling region. If a 1% pressure oscillation ($\Delta p/p = 0.01$) is allowed, then $O(100)$ grid points are needed to resolve this jump. The typical length scale of the interface in practical applications is $O(0.1 \text{ mm})$ for transcritical flows [41,46], so that an $O(1 \mu \text{m})$ grid resolution will be required. Note that for ideal gas flows, the jump in $1/(\gamma^* - 1)$ is an order of magnitude smaller than for transcritical flows given the same range of temperature, as can be seen in Fig. 2(b). Therefore, the significant jump between liquid-like and gas-like fluid results in the large jump in $\gamma^*$ which causes significant spurious pressure oscillations in the transcritical regime.
The occurrence of spurious pressure oscillations is known for multi-species calorically perfect gas flows and reacting systems for ideal gas. For ideal gas flows, under certain conditions no special treatment other than artificial diffusion is adopted to suppress these oscillations [47]. Until recently, several transcritical simulations with fully conservative schemes are reported to suffer from pressure oscillations, preventing simulations of cryogenic fuel injection [10,12–15]. Terashima and Koshi [13] developed and solved the pressure evolution equation for real fluids instead of the total energy equation in a finite difference approach based on the work of [48] for calorically perfect gas flows. However, it is not straightforward to extend this approach to finite-volume methods since pressure is not a conserved quantity, a Riemann solver is not available for the system with the pressure evolution equation, and this method needs significant modification to an existing solver. These constraints motivate the development of the following double-flux model for transcritical simulations.

4.2. Double-flux model

The principle of the double-flux model is based on the results from Eq. (19). Since spurious pressure oscillations arise whenever \( \gamma^* \) or \( c_0^e \) are not constant, the main idea of the double-flux model is to freeze \( \gamma^* \) and \( c_0^e \) both in space and time during each time-step advancement [11,22].

For clarity, we consider first a one-dimensional case to derive the model. This model is subsequently extended to multidimensions. The numerical flux for the face at \( x_{j+\frac{1}{2}} \) can be expressed as

\[
F_{j+\frac{1}{2}}^e = F^e(U_{j+\frac{1}{2}}^L, U_{j+\frac{1}{2}}^R),
\]

where \( U_{j+\frac{1}{2}}^L \) and \( U_{j+\frac{1}{2}}^R \) are the left and right reconstructed states at the face \( x_{j+\frac{1}{2}} \), computed from the corresponding stencils. The first step in the double-flux model is to compute and store \( \gamma^* \) and \( c_0^e \) for each computational cell. Denoting \( S_{j+\frac{1}{2}} \) to be the set of cells in the stencil belonging to face \( x_{j+\frac{1}{2}} \), see Fig. 3. Two fluxes are computed for the same face \( x_{j+\frac{1}{2}} \), which are \( F_{j+\frac{1}{2}}^{e,L} \) for cell \( j \) and \( F_{j+\frac{1}{2}}^{e,R} \) for cell \( j+1 \). As an example, during the reconstruction process for face \( x_{j+\frac{1}{2}} \), whenever the total energy in the stencil is needed, the value is computed from \( \gamma^* \) and \( c_0^e \) for cell \( j \) through

\[
(p_{el})_l^n = \frac{p_l^n}{\gamma_j^{n,n} - 1} + p_l^n c_{0,0,j}^n + \frac{1}{2} p_l^n u_l^n \cdot u_l^n,
\]

where \( l \in S_{j+\frac{1}{2}} \). If primitive variables are used for the reconstruction, this step is only applied when the flux at the face is computed from primitive variables. For example, if a Riemann flux is used, the total energy of the left and right states is evaluated from Eq. (21). It can be seen that the numerical flux for the energy at face \( x_{j+\frac{1}{2}} \) will be different for cells \( j \) and \( j+1 \) since different values of \( \gamma^* \) and \( c_0^e \) are used.

After the conservative variables are updated, the primitive variables for each cell are updated using the values of \( \gamma^* \) and \( c_0^e \). Specifically, the pressure is updated using the following expression for cell \( j \).

\[
p_{j+1}^{n+1} = (\gamma_j^{n,n} - 1) \left( (p_{el})_{j+1}^{n+1} - p_{j+1}^{n+1} c_{0,0,j}^{n+1} - \frac{1}{2} p_{j+1}^{n+1} u_{j+1}^{n+1} \cdot u_{j+1}^{n+1} \right).
\]

This step ensures that \( \gamma^* \) and \( c_0^e \) are frozen for cell \( j \) in time.
The treatment in the double-flux model reduces each cell to represent a calorically perfect gas with constant specific heat ratio, so that spurious pressure oscillations are eliminated. The procedure for time advancement from time $t^n$ to $t^{n+1}$ using the double-flux model developed in the current study is summarized in Algorithm 1. Note that the last step in the algorithm is essential to ensure that the final thermodynamic state is consistent between primitive and conservative quantities. A MATLAB code with the double-flux model implemented is provided in Appendix D as a reference example. Algorithm 1 shows that the procedure using the double-flux model is similar to the conventional fully conservative schemes, and only requires modifications to transform between total energy and pressure. The computational overhead for the scheme using the double-flux model is the cost to compute an additional flux of total energy for each cell.

In the procedure above, the effective specific heat ratio, $\gamma^*$, is evaluated from Eq. (12) which is based on the thermodynamic speed of sound. Since for each cell the system is represented by a calorically perfect gas, the characteristic speed of sound of the Euler system becomes equal to the thermodynamic speed of sound, and this is consistent with the characteristics of the original Euler system.

An added benefit of the procedure using the double-flux model over the conventional fully conservative method is that the iterative procedure typically involved when a cubic EoS is used can be avoided. Figure 4 shows the flow charts for updating primitive variables given conservative variables (Step 3 in Algorithm 1) for both the fully conservative method and the double-flux model. For a fully conservative scheme, the internal energy and species can be determined from conservative quantities in a straightforward manner. Then pressure or temperature need to be determined iteratively from density, energy and species since for cubic EoS, the internal energy is a complex nonlinear function of thermodynamic states (see Eq. (39)). Although a Newton-type iterative solver can be applied, this iterative procedure is usually costly since it has to be done for each cell. In contrast, for the numerical scheme in which the double-flux model is applied, the pressure can be directly obtained from Eq. (22). For cubic EoS, the temperature can be determined analytically given density, pressure and species as outlined in Appendix C. Therefore, costly iterative procedures can be avoided. Note that for more complex EoSs, an analytic solution for temperature from density, pressure and species may not be available.

Although mass, momentum, and species are conserved for finite-volume schemes, the double-flux model introduces an energy conservation error. Similar to the case for calorically perfect gas [11], the energy conservation error results from the freezing of thermodynamic relations. The resulting error in the energy conservation can be evaluated by considering a contact interface in which the conservation equations are discretized using a first-order upwinding flux. Due to the freezing of thermodynamic relations in space, the error after one time step at the face at $x_{j+1/2}$ can be expressed as

$$
\epsilon_{\text{space}} = \Delta t \left[ F_{j+1/2}^e R - F_{j+1/2}^e L \right] = \Delta t \left[ u p \Delta \left( \frac{1}{\gamma^* - 1} \right) + \rho u \Delta \epsilon_0^* \right],
$$

where $F_{j+1/2}^e L$ and $F_{j+1/2}^e R$ are the double fluxes at face $x_{j+1/2}$. The conservation error due to the freezing of the thermodynamic relations in time for cell $j$ is
\[ \epsilon_{\text{time}} = \Delta x \left[ (\rho e_1|_{\gamma^* = \phi^* = 0} - (\rho e_1)|_{\gamma^* = \phi^* = 1}) = -\Delta x \left[ \frac{1}{\gamma^* - 1} \right] + \rho^{n+1} \delta e_0^* \right]. \] (24)

This error is introduced during the last step when the total energy is updated in Algorithm 1. It can be seen that the energy conservation error depends on the jump in \(1/(\gamma^* - 1)\) and \(\epsilon_0^*\). For smooth solutions, it can be inferred that the jump related to \(\gamma^*\) and \(\phi^*\) will decrease as \(\Delta x\) decreases. Numerical tests will be conducted in Section 5.1 to evaluate the conservation error associated with the currently developed high-order numerical scheme. Note that although strong shocks are not expected in rocket motors, gas turbines or diesel engines, the double-flux model has been shown to have excellent performance even in the presence of strong shock waves [11,25].

4.3. Entropy-stable hybrid scheme

The numerical capability developed in the present work aims to study real-fluid physics in practical engineering devices. For these applications, high-Reynolds number flows are generally turbulent and can strongly affect the dynamics of interfaces, mixing and subsequent chemical reactions. Therefore, the turbulent flow behavior needs to be accurately represented. Numerical methods to facilitate large-eddy simulation (LES) and direct numerical simulation (DNS) techniques have been investigated in previous studies [28,29], and the importance of using non-dissipative schemes was emphasized in [49]. In the present study, a reconstruction-based finite-volume scheme with hybrid flux is employed [50]. For hexahedral meshes, the high-order polynomial reconstruction retains fourth-order accuracy on uniform meshes and third-order accuracy on non-uniform meshes. However, it is noted that purely non-dissipative schemes often suffer from numerical instabilities, for compressible flow problems, especially with strong turbulence [51]. Therefore, the non-dissipative scheme is augmented with a second-order ENO scheme [52], which is applied in an adaptive manner.

The important ingredient of the hybrid scheme is an appropriate sensor, which is used to determine the region where the dissipative scheme is applied. There are a variety of different types of sensors available in the literature. For transcritical simulations, which are characterized by large density gradients, numerical difficulties arise in regions where sharp density gradients occur. Therefore, a natural choice for the sensor is to utilize the density field. A relative solution (RS) sensor [50] is used in the present study. For each control volume (CV), the RS-sensor determines whether the face density value from high-order non-dissipative reconstruction, \(\rho_f\), and the density value at the CV-center, \(\rho_{CV}\), differs by more than some fraction of the density at the CV-center. This relation can be expressed as:

\[ \left| \frac{\rho_f - \rho_{CV}}{\rho_{CV}} \right| > \zeta, \]

(25)

where \(\zeta\) is a user-input parameter. In the following, the effects of the RS-parameter \(\zeta\) on the numerical solution will be examined through numerical tests. This smoothness indicator is simply the difference between the reconstructed face value and the upwind CV value, and can therefore be implemented very efficiently. The scheme maintains the conservative property of the underlying finite-volume scheme. The described hybrid scheme has been successfully used for simulations of various applications for ideal gas flows [53–55]. For this reason, we will consider this method as baseline discretization for the flux formulation.

Although the baseline scheme introduced above shows good performance for predicting turbulence of ideal gases, the scheme is still not sufficiently robust for the prediction of transcritical turbulent flows, due to the existence of sharp density profiles and strong nonlinear coupling of thermodynamic variables. Non-physical solutions, such as negative pressure or density, or unbounded mass-fractions, often appear during the solution process. Due to large density gradients, unrealizable solutions occur on under-resolved meshes. To address this issue, we appeal to utilize the concept of an entropy-stable flux formulation, which preserves the physical realizability of numerical solutions [30,31]. To this end, we combine the original scheme with a flux correction step. Based on the study of Tadmor [30,56], the Lax–Friedrichs flux formulation is selected as the low-order flux. This flux reads:

\[ F^{e,LF}_{j+\frac{1}{2}} = \frac{1}{2} \left[ F(U_j) + F(U_{j+1}) \right] - \frac{\lambda}{2} (U_{j+1} - U_j), \quad \text{where} \quad \lambda = \max_{j,j+1} |u| + c \]

(26)

refers to the local maximum characteristic speed. It was shown that this flux formulation is able to preserve positivity of pressure and density, ensures the boundedness of species mass fractions, and enforces entropy boundedness [30,57].

In the proposed procedure, the numerical solution is first advanced using the non-dissipative hybrid flux scheme, followed by an a posteriori check. In regions where the solution violates the density, pressure, mass fraction or entropy realizability, a correction step is applied, by which the local solution is corrected using the low-order entropy-stable flux. The detection criterion is naturally constructed according to the discrete minimum entropy principle [56]:

\[ s(U_j^{k+1}) > s_{\text{min}} = \min_{i \in \text{nb}(j)} s(U_i^k), \]

(27)

where the superscript \(k\) refers to stage \(k\) in the RK-scheme, and \(\text{nb}\) refers to the neighboring cells of the local cell. The principle was initially proposed by Tadmor [56] and further extended for discontinuous Galerkin schemes [31,57].
Algorithm 2: Procedures for entropy-stable (ES) flux correction.

Evaluate entropy bound: For each cell, find entropy bound $s_{\text{min}}$ according to Eqs. (27) and (28);
for each stage $k$ of Runge–Kutta scheme do
  Step 1: Update solution vector $U^k \to U^{k+1}$ with numerical flux from the hybrid scheme;
  Step 2: For each cell, examine if the solution violates the criterion given in Eq. (27). If so, mark the cell as a troubled cell;
  Step 3: For troubled cells and their neighbors, correct the solutions by the difference between the low-order flux (Eq. (26)) and the original flux;
  Step 4 (optional): Go to step 2.
end

Table 1
Molecular weight, acentric factor, and critical properties for temperature, pressure, density, and compressibility for different species considered in the test cases.

<table>
<thead>
<tr>
<th>Species</th>
<th>$W$ [kg/kmol]</th>
<th>$\omega$</th>
<th>$T_c$ [K]</th>
<th>$p_c$ [MPa]</th>
<th>$\rho_c$ [kg/m$^3$]</th>
<th>$Z_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N$_2$</td>
<td>28.0</td>
<td>0.0372</td>
<td>126.2</td>
<td>3.40</td>
<td>313.3</td>
<td>0.289</td>
</tr>
<tr>
<td>O$_2$</td>
<td>32.0</td>
<td>0.0222</td>
<td>154.6</td>
<td>5.04</td>
<td>436.1</td>
<td>0.287</td>
</tr>
<tr>
<td>H$_2$</td>
<td>2.02</td>
<td>–0.219</td>
<td>33.15</td>
<td>1.30</td>
<td>31.26</td>
<td>0.303</td>
</tr>
<tr>
<td>n-C$<em>{12}$H$</em>{26}$</td>
<td>170.3</td>
<td>0.574</td>
<td>658.1</td>
<td>1.82</td>
<td>226.5</td>
<td>0.249</td>
</tr>
</tbody>
</table>

Table 2
Summary of spatial dimensionality, system solved, and sub-grid scale model of the test cases.

<table>
<thead>
<tr>
<th>Test case</th>
<th>Section</th>
<th>Dimensionality</th>
<th>System</th>
<th>Sub-grid scale model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Advection of nitrogen interface</td>
<td>Section 5.1</td>
<td>1D</td>
<td>Euler</td>
<td>-</td>
</tr>
<tr>
<td>Transcritical shock tube problem</td>
<td>Section 5.2</td>
<td>1D</td>
<td>Euler</td>
<td>-</td>
</tr>
<tr>
<td>Advection of n-dodecane drop</td>
<td>Section 5.3</td>
<td>2D</td>
<td>Euler</td>
<td>-</td>
</tr>
<tr>
<td>Nitrogen injection</td>
<td>Section 5.4</td>
<td>2D</td>
<td>Navier–Stokes</td>
<td>none</td>
</tr>
<tr>
<td>LOX/GH2 mixing</td>
<td>Section 5.5</td>
<td>2D</td>
<td>Navier–Stokes</td>
<td>none</td>
</tr>
<tr>
<td>Cryogenic nitrogen injection</td>
<td>Section 5.6</td>
<td>3D</td>
<td>Navier–Stokes</td>
<td>Vreman</td>
</tr>
</tbody>
</table>

A smooth convex function of flow variables augmented with an entropy flux can be considered as a generalized entropy function of a hyperbolic system [30]. The physical entropy that is consistent with the state equation (Eq. (41)) can be considered as one candidate. When the double-flux model is used, which essentially formulates the system as a calorically perfect gas representation with a constant specific heat capacity ratio, the ideal-gas entropy formulation can be adopted using the effective specific heat ratio $\gamma^*$:

$$ s = \ln \left( \frac{p}{(\rho R)^{\gamma^*}} \right) + (\gamma^*-1) \sum_{i=1}^{N_s} X_i \ln X_i, \quad (28) $$

where $X_i$ is the mole fraction of species $i$. Note that the positivity of density, pressure and the boundedness of mass fractions between zero and one are embedded in Eq. (28).

The implementation of the entropy-stable hybrid scheme is summarized in Algorithm 2. After troubled cells are identified, the difference between the low-order flux and the original flux from the hybrid scheme is added to the trouble cell instead of re-updating the solution from the state at the previous stage. The region in which the entropy condition is violated should be local and the flux correction procedure adds minimal overhead to the original numerical scheme. To preserve conservation properties, the flux correction should also be applied at the contiguous face of the neighbor cells. Since for a neighboring cell, not all of its faces are updated using the low-order flux, the entropy boundedness cannot be guaranteed, and therefore an iterative procedure needs to be applied. However, it was found through numerical experiments that usually only one correction was needed to ensure the entropy boundedness for all cells in the computational domain. Note that this procedure is not limited to hybrid schemes, and it can also be used to correct other types of numerical fluxes when they violate the discrete minimum principle.

5. Numerical tests

A series of test cases are considered to demonstrate the capability of the developed numerical scheme. All test cases are performed using an unstructured finite-volume code, CharlesX, which has been developed at the Center for Turbulence Research at Stanford University. In these test cases, flows with different species are considered, which are relevant for practical applications. The critical properties of the species considered in this study are listed in Table 1. Table 2 summarizes the dimensionality, system solved, and sub-grid scale models used for the test cases considered.
5.1. One-dimensional advection of nitrogen interface

A one-dimensional advection configuration is selected to evaluate the performance of the proposed numerical schemes. Note that the Euler system is solved for all test cases in this subsection, which enables a direct comparison with analytical solutions.

The test case involves nitrogen as the working fluid. The pressure is set to 5 MPa, which is above the critical pressure of nitrogen. The computational domain is \( x \in [0, 1] \) m and a uniform mesh with 150 grid points is used. Periodic boundary conditions are applied.

Two types of initial conditions are considered. One case involves a sharp jump of density, and the other case considers a smooth density profile. For the case with the sharp density jump, the initial conditions are

\[
\rho = \begin{cases} 
\rho_{\max}, & 0.25 \text{ m} < x < 0.75 \text{ m} \\
\rho_{\min}, & \text{otherwise}
\end{cases}
\]  

(29)

For the case with smooth density profile, a harmonic wave is given for the density with the same maximum and minimum as for the case with a sharp jump initial condition,

\[
\rho = \frac{\rho_{\min} + \rho_{\max}}{2} + \frac{\rho_{\max} - \rho_{\min}}{2} \sin(2\pi x).
\]  

(30)

The two states of nitrogen correspond to \( T_{\min} = 100 \text{ K}, \rho_{\max} = 793.1 \text{ kg/m}^3 \) and \( T_{\max} = 300 \text{ K}, \rho_{\min} = 56.9 \text{ kg/m}^3 \), respectively. For all computations, the CFL-number is set to a value of 0.8. The advection velocity is 100 m/s for all cases and the simulation is run for one period, corresponding to a physical time of 0.01 s.

Figure 5 shows results for density, temperature, specific internal energy, and pressure for the case with a sharp jump initial condition. The exact solution for this case is the advection of the initial condition with constant pressure and velocity.

To examine the behavior of the hybrid scheme, simulations with different threshold values of the RS-sensor are performed. Results with and without the entropy-stable flux correction for \( \zeta = 0.2 \) are both presented to illustrate the effect of the entropy stability. As can be seen in the pressure profiles in Fig. 5, the present numerical scheme with the double-flux model preserves the pressure and velocity equilibrium (not shown) without generating spurious oscillations. In contrast, the fully conservative scheme will fail the simulation at the first sub-iteration of the SPP-RK3 time advancement due to the
negative pressure that is generated from the strong oscillations as a result of the large discontinuity in $\gamma^*$ and $e_0^*$. Refining the grid will not solve the problem unless the initial condition is smooth and can be fully resolved.

The effect of using different sensor values in the hybrid scheme is clearly seen in the density and temperature profiles in Fig. 5. Primitive variables are used for the reconstruction in the ENO scheme for all test cases in this study and no significant difference was observed using reconstruction from conservative variables. For the case with $\xi = 0$, the ENO scheme is applied everywhere in the computational domain, and the results do not show any visible oscillations. As the sensor value is relaxed, the solution for density and temperature becomes less diffusive and the interface becomes sharper, but small oscillations in density become apparent. Due to the non-linearity in the thermodynamics, oscillations introduced by numerical instabilities are subsequently magnified in the temperature profiles. For $\xi = 0.2$ the results with the entropy-stable flux are also included for comparisons. It can be seen that density overshoots are eliminated. Undershoots in density are also dampened. The results are similar to that in [31], which shows that the herein proposed entropy-stable scheme has the ability to dampen oscillations across the contact interface.

To quantify the effect of the entropy-stable flux and the behavior of different sensor values, a series of tests with discontinuous initial conditions are conducted using different sensor values. Maximum overshoots and undershoots in density are studied along with the numerical interface thickness, $I_\rho$, which is defined as [10]:

$$I_\rho = \frac{l_\rho}{\Delta x} = \frac{\Delta \rho}{\Delta x \left. \frac{\partial \rho}{\partial x} \right|_{\max}},$$

(31)

where $\Delta \rho$ is the jump across the interface. The derivative in density is computed using a second-order finite difference approximation. A uniform mesh with 150 grid points is used. The results are shown in Fig. 6. RS-sensor values tested range from 0 to 0.6. As can be seen from Fig. 6, overshoots and undershoots for the cases without entropy-stable flux increase as less diffusion is introduced. On the other hand, with the entropy-stable flux applied, the overshoots are eliminated and have a value of almost zero. The undershoots are also dampened by a factor of two compared to the cases without entropy-stable flux. For the interface representation, the interface thickness initially remains constant for $\xi \leq 0.1$, and starts to decrease as $\xi$ increases. The entropy-stable flux correction maintains the sharpness of the contact discontinuity. Results with $\xi = 0.2$ and entropy-stable flux yield a sharp interface with acceptable density variations, therefore all the following test cases are conducted with this sensor value.

Figure 7 shows results of the convergence study of the current numerical scheme for initial conditions with sharp and smooth density profiles. Results for $L_2^*$- and $L_\infty$-errors of density with and without the entropy-stable flux are shown. As can be seen, first-order convergence is observed on sharp discontinuous initial conditions and the current numerical scheme retains fourth-order accuracy on smooth solutions, regardless of whether an entropy-stable flux is applied.

To examine the conservation property of the double-flux model, the evolution of the energy conservation error is evaluated for the cases with discontinuous and smooth initial conditions. The energy conservation error is defined as

$$\varepsilon = \left| \frac{\int_{\Omega} (\rho e) t(t) dx - (\rho e)(0) \right| dx}{\int_{\Omega} (\rho e)(0) dx},$$

(32)

which is the relative error of the total energy with respect to initial conditions and $\Omega$ represents the computation domain. Results with $\xi = 0.2$ using the entropy-stable flux are shown in Fig. 8. Results with other RS-sensor values and without the entropy-stable flux correction produce similar behavior, and are therefore omitted. For all cases, the conservation error initially increases rapidly and subsequently approaches a plateau. This is similar to the findings from previous studies [11]. For the case with discontinuous initial condition, the conservation error at the end of one period shows a first-order mesh
Fig. 7. Grid convergence study for the one-dimensional N₂ advection case with (a) sharp jump initial condition, and (b) smooth initial profile. The RS-sensor is set to 0.2 for all cases.

Fig. 8. Energy conservation error for the one-dimensional N₂ advection case for (a) sharp jump initial condition, and (b) smooth initial profile. ζ = 0.2 with entropy-stable flux applied.

convergence. While for the case with smooth profile of density, a much faster convergence can be observed. This is due to the fact that for smooth solutions, the profiles of γ* and e*₀ are also smooth and as the mesh is refined, the jump in thermodynamic properties is reduced in addition to the decrease in the mesh size Δx. Mass and momentum are conserved by the current numerical scheme to the level of machine accuracy. Overall, the conservation error in total energy of the current numerical scheme with double-flux model is acceptable and converges to zero with mesh refinement.

5.2. Transcritical shock tube problem

In this subsection, a transcritical shock tube problem is considered. Simulations are performed using both the fully conservative scheme, and the quasi-conservative scheme with the double-flux model applied to the Euler system. The computational domain is x ∈ [0, 1] m and a uniform mesh is utilized. Solid adiabatic wall boundary conditions are applied at the boundaries. Nitrogen is considered as the working fluid. The initial conditions are

\[
\begin{pmatrix}
\rho_L \\
\rho_L u_L \\
\end{pmatrix} = \begin{pmatrix}
800 \text{ kg/m}^3 \\
60 \text{ MPa} \\
0 \\
\end{pmatrix}, \quad \begin{pmatrix}
\rho_R \\
\rho_R u_R \\
\end{pmatrix} = \begin{pmatrix}
80 \text{ kg/m}^3 \\
6 \text{ MPa} \\
0 \\
\end{pmatrix},
\]

where the initial jump is placed at x = 0.5 m. A reference simulation is obtained using a fully conservative scheme on a uniform mesh with 50,000 grid points and pure ENO scheme (ζ = 0). For the results with the double-flux model, the hybrid scheme described previously is utilized for the simulations with the RS-sensor set to a value of 0.2. Entropy-stable flux is applied and its effect on the contact interface will be studied. A CFL-number of 0.8 is used for all test cases and the simulations are time advanced until t = 5 × 10⁻⁴ s.
Fig. 9. Results of density, velocity, pressure, and temperature for the transcritical shock tube problem at $t = 5 \times 10^{-4}$ s for different mesh resolutions. The RS-sensor is set to $\zeta = 0.2$ for all cases and entropy-stable flux is applied.

Figure 9 shows results for density, velocity, pressure, and temperature for the shock tube problem using the double-flux model with different mesh resolutions. Results from the fully conservative scheme are shown for comparisons. It can be seen that the current numerical scheme captures the essential features of the shock tube problem. Specifically, no oscillations in density and temperature are observed across the contact interface. Due to the energy conservation error, faster shock speed predictions can be observed on coarse meshes, and this improves with increasing mesh resolution. This is also seen in the work by Pantano et al. [21] if a Roe solver is used. Small overshoots/undershoots in velocity and pressure can be seen at the shock and the expansion fan, although the magnitude decreases with increasing resolution. The reason for the fluctuations is probably due to the primitive reconstruction and can be addressed with a reconstruction using characteristic variables [52].

Figure 10 shows the conservation properties for the shock tube problem. Similar to the nitrogen advection case with a sharp initial profile (Section 5.1), the small conservation error exhibits a first-order convergence behavior.

Fig. 10. Energy conservation error as a function of time for the transcritical shock tube problem. $\zeta = 0.2$ with entropy-stable flux applied.
Fig. 11. Results of density profiles for the transcritical shock tube problem with and without the entropy-stable flux applied. \( N = 512 \) and \( \zeta = 0.2 \). ES refers to the entropy-stable flux formulation.

**Fig. 12.** Schematic and boundary conditions of the two-dimensional advection case of a \( n \)-dodecane drop.

Figure 11 shows the density profiles using a mesh of 512 grid points with the contact interface region zoomed in. Results with and without entropy-stable flux correction technique are shown for comparison. The RS-sensor is set to the same value of 0.2 for both cases. It can be seen from Fig. 11 that without the entropy-stable flux, the hybrid scheme shows oscillatory behavior across the contact interface even with high resolution; however, the entropy-stable flux dampens the oscillations across the interface. This is similar to the findings by Zhang and Shu [31].

The shock tube problem with ideal-gas EoS has been studied extensively using the double-flux model by Abgrall and Karni [11], where simulation results are in excellent agreement with exact solutions even for severe test conditions. Although the present study mainly focuses on contact discontinuities, it is shown that the developed numerical scheme is capable of also handling shock waves under transcritical conditions.

5.3. Two-dimensional advection of \( n \)-dodecane drop

To study the performance of the numerical scheme for multi-species flows, a two-dimensional test case is considered, which involves the advection of an \( n \)-dodecane drop. The schematic and boundary conditions of this test case are shown in Fig. 12. An \( n \)-dodecane liquid drop at a temperature of 363 K is initially placed in the center of the domain in a 900 K nitrogen environment. The pressure is set to 6 MPa. This condition corresponds to the Spray A operating point [46]. Note that the pressure is above the critical condition for both species. The computational domain is a square with a length of 1 mm, which is twice the diameter of the liquid drop. A uniform mesh of 100 \( \times \) 100 cells is used. The advection speed is set to 50 m/s. The Euler system is solved and the CFL-number is set to a value of 0.8.

Figure 13 shows the profiles for density and fuel mass fraction at the centerline in the \( y \)-direction after one period at \( t = 0.02 \) ms. Results with and without the entropy-stable flux are shown in comparison with the exact solution. Pressure and velocity maintain equilibrium with the double-flux model as for the single-species case. The effect of the entropy-stable flux on damping the numerical oscillations is similar to that for the single-species case. Without the entropy-stable flux, numerical oscillations due to nonlinear instabilities result in negative mass fractions of \( n \)-dodecane as can be seen in Fig. 13. Although the negative mass fraction can be clipped to within the bounds, the conservation of each species will not be
maintained. The mass fraction here is left with negative values intentionally to show the effect of the entropy-stable flux correction. As can be seen, the entropy-stable flux ensures that mass fractions are within their physical bounds.

5.4. Two-dimensional nitrogen injection

A two-dimensional cryogenic planar jet mixing case is simulated to demonstrate the multidimensional capability of the current numerical scheme. A schematic of the computational setup is illustrated in Fig. 14. A cryogenic nitrogen jet at 80 K is injected into a nitrogen vessel at a temperature of 300 K. The ambient pressure is initially set to be constant at 4 MPa, corresponding to a transcritical mixing case. Note that in the present study the Navier–Stokes system is solved. The transport models used in this test case are described in Section 3.2. The height of the jet exit nozzle is $h = 1.0$ mm and the jet velocity is set to a value of 100 m/s, which corresponds to a Reynolds number of $5.2 \times 10^5$ and a Mach number of 0.12. A domain of $30h \times 16h$ is used. A uniform mesh in both directions is employed, having a spacing of 0.02$h$ with 50 grid points across the jet. The inlet condition of the jet is a plug flow with a top-hat velocity profile. Periodic boundary conditions are applied at the top and bottom boundaries, and an adiabatic no-slip wall condition is applied at the left boundary. The pressure is specified at the outlet at the right boundary. This configuration is similar to the test case studied in [13]. The operating conditions are slightly more challenging compared to the previous study since this test case contains a discontinuous inlet profile and smoothing is not applied. The hybrid scheme using the double-flux model with RS-sensor set to $\zeta = 0.2$, and the entropy-stable flux is applied. The CFL-number is set to a value of 1.0. No subgrid scale model is used in this case since the purpose of this test case is to examine the performance of the current numerical scheme.

Figure 15 shows results for density, temperature, pressure and speed of sound at $t = 3.96$ ms, right before the jet reaches the end of the domain. No spurious pressure oscillations are generated in this case. For a fully conservative scheme on the same mesh, the simulation will diverge due to large pressure oscillations within several iterations. This was also observed in [13] and in our previous simulations [15]. The code divergence can be avoided by employing a very fine mesh and using a smooth inlet profile so that the fully conservative scheme can resolve the difference in $\gamma^*$ and $e_h^*$ to the extent that the numerical dissipation inherent in the scheme can suppress spurious pressure oscillations. However, this is not feasible in practical applications, especially when LES-techniques are considered. With the double-flux model, pressure oscillations do not show up even on a mesh that is coarsened by two levels. Note that the current resolution is not sufficient to resolve all small-scale structures in the flow field, and in practical 3D-simulations, a subgrid scale model would be used to model the turbulence effects.
Fig. 15. Instantaneous fields of density, temperature, pressure and speed of sound for the two-dimensional N₂ injection case at \( t = 3.96 \) ms. Ranges in legends are not adjusted.

Fig. 16. Instantaneous fields of temperature with and without entropy-stable flux for the two-dimensional N₂ injection case at \( t = 3.96 \) ms. Zoomed-in region of the domain is shown. Ranges in legends are not adjusted.

The ranges in the legends of Fig. 15 are not adjusted to show the capability of the current numerical scheme to suppress the numerical oscillations while maintaining the sharp interface associated with the transcritical flow. With entropy-stable flux applied, the amount of overshoot/undershoot in density and temperature are similar to that seen in the one-dimensional test cases in Section 5.1. Due to the entropy-stable flux correction technique, undershoots in temperature are negligible while small overshoots are present. For comparison, Fig. 16 shows temperature fields with and without entropy-stable flux correction at the same physical time. A zoomed-in region is shown. As can be seen in Fig. 16(b), although the hybrid scheme with RS-sensor ensures the robustness of the simulation, overshoots and undershoots are more pronounced compared to the results shown in Fig. 16(a). This is similar to the finding from the one-dimensional test cases.
5.5. Two-dimensional LOX/GH2 mixing

To demonstrate the capability of the newly developed numerical scheme, a two-dimensional mixing layer, consisting of liquid–oxygen (LOX) and gaseous–hydrogen (GH2) streams, is simulated. This case was proposed in [41] as a benchmark case to test numerical solvers for high-Reynolds number turbulent flows with large density ratios. The configuration and boundary conditions are shown in Fig. 17. The configuration is representative of a coaxial rocket combustor, in which dense LOX is injected in the center to mix with the surrounding high-speed GH2 stream. The two streams are separated by the injector lip, which is also included in the computational domain. A domain of 15h × 10h is used, where h = 0.5 mm is the height of the injector lip. The origin is set at the center of the lip face. The region of interest extends from 0 to 10h in the axial direction, with a sponge layer of length 5h at the end of the domain. A grid convergence study was conducted in [41], showing that for the mesh with 100 grid points across the injector lip, the statistics do not show noticeable differences with further refinement. Therefore, this resolution is used in the current study. A fully structured Cartesian mesh is utilized in this case. A uniform mesh is used in both directions for the region from 0 to 10h in axial direction and from −1.5h to 1.5h in transverse direction; stretching is applied with a ratio of 1.02 only in the transverse direction outside of this region. The mesh is stretched in axial direction in the sponge layer. This results in a mesh with a total of 5.2 × 10^7 cells.

Adiabatic no-slip wall conditions are applied at the injector lip and adiabatic slip wall conditions are applied at the top and bottom boundaries of the domain. A 1/7th power law for velocity is used for both the LOX and GH2 streams. Pressure outlet boundary conditions are applied after the sponge layer where spurious acoustic waves are suppressed. The LOX stream is injected at a temperature of 100 K, and GH2 is injected at a temperature of 150 K. The pressure is set to 10 MPa which is representative of rocket combustor conditions. Note that the density ratio between LOX and GH2 is about 80. The Reynolds numbers, defined using the lip height and injection velocities, are 5 × 10^4 and 2 × 10^5, and Mach numbers are 0.03 and 0.12, for the oxygen and hydrogen streams, respectively. The Navi–Stokes system is solved with transport quantities obtained through models described in Section 3.2. The hybrid scheme using the double-flux model with entropy-stable flux correction is used and the R5-sensor is set to a value of 0.2. A first-order upwinding scheme is used in the sponge layer. The CFL-number is set to 1.0 and no subgrid scale model is used to facilitate comparisons with the results in [41].

Figure 18 shows results for instantaneous axial velocity, transverse velocity, oxygen mass fraction and density. No spurious pressure or velocity oscillations are seen during the simulation and the sponge layer efficiently absorbs the outgoing acoustic waves. The flow field is dominated by large vortical structures in the mixing layer. As can be seen from Fig. 18, three large vortical structures are separated by waves with a wavelength of approximately 5h. The predicted structures of vortices are in good agreement with those reported in [41]. From the density field, “comb-like” or “finger-like” structures [3, 14] can clearly be seen, which was also observed through experiments for transcritical mixing under typical rocket engine operating conditions [1,3,4]. The current numerical scheme is capable of capturing sharp density gradients in this flow with very large density ratios robustly while resolving the sharp interface without numerical difficulties.

To further assess the simulation results, the flow field was averaged over 15 flow-through-times after reaching steady state, with one flow through time corresponding to 0.125 ms [41]. This time period was shown to be sufficient to obtain converged statistics. Mean and root-mean-square (rms) results for axial velocity, transverse velocity, temperature, and oxygen mass fraction are shown in Figs. 19 to 22. Statistics at different axial locations (x/h = 1, 3, 5, 7) are plotted as a function of normalized transverse distance. Results are compared to those obtained from two other numerical solvers, namely AVBP and RAPTOR [41]. A mesh of 250 grid points across the injector lip was used for AVBP and RAPTOR, which is 2.5 times finer than the mesh used in the present study. The mean axial velocity is in good agreement between the three different solvers, while there are some discrepancies in the rms values. Results from CharlesX show slightly lower rms values on the GH2 side, especially for the axial location of x/h = 3. This is probably due to the different implementation of the sponge layer and outlet boundary conditions adopted by the different solvers [58]. For the transverse velocity, a similar behavior is observed among three solvers due to the coupling between velocities in two directions. The magnitude of the transverse velocity is much smaller than that of the axial velocity so that the difference in the mean values can be seen clearly. Results for the oxygen mass fraction are almost identical for the three solvers except for the small difference seen at the GH2 side which could be related to the difference seen in the velocity results. Appreciable differences are seen in the
temperature statistics in Fig. 22. The results from CharlesX and AVBP are similar and show a narrower thermal mixing layer as compared to that of RAPTOR.

The spatial evolution of the mixing layer thickness in the axial direction from three different solvers is shown in Fig. 23. The thickness of the mixing layer at a given axial location is defined as the distance between the locations where the oxygen mass fraction deviates from zero and unity. Results from two criteria are plotted ($Y_{O2} = 0.01, 0.99$ and $Y_{O2} = 0.05, 0.95$). The results from CharlesX are in good agreement with the results from the other two solvers. CharlesX produces a lower value of the thickness with the criterion that has a threshold value of 1%. For the criterion with a threshold value of 5%, CharlesX shows similar behavior as AVBP. These results are consistent with the results in Fig. 21.

5.6. Cryogenic nitrogen injection

The test cases in this subsection examine the performance of the present numerical scheme in three dimensions in the context of LES. To this end, the cryogenic nitrogen injection cases of Mayer et al. [59] are considered. In the experiment, a cryogenic supercritical nitrogen jet is injected into an ambient nitrogen reservoir at 298 K and 3.97 MPa. Cases 3 and 4
Fig. 19. Transverse cuts of (a) mean and (b) rms axial velocity of the two-dimensional LOX/GH2 mixing case.

Fig. 20. Transverse cuts of (a) mean and (b) rms transverse velocity of the two-dimensional LOX/GH2 mixing case.

Fig. 21. Transverse cuts of (a) mean and (b) rms oxygen mass fraction of the two-dimensional LOX/GH2 mixing case.

in this experimental campaign are simulated, corresponding to injection conditions of 126.9 K, 440 kg/m$^3$ and 131 K, 170 kg/m$^3$, respectively. The injection speeds are 4.9 m/s and 5.4 m/s for Cases 3 and 4, respectively, corresponding to Reynolds numbers of $1.7 \times 10^5$ and $1.6 \times 10^5$ and Mach numbers of 0.02 and 0.024.

Figure 24 displays the schematic of the computational domain. A cylindrical domain is adopted and no inlet pipe is included. The injector diameter, $d$, is 2.2 mm and the dimensions of the domain are the same as in the experiment. Cryogenic nitrogen is injected with a plug-flow profile and no smoothing or turbulence profile is used. Isothermal no-slip conditions are applied at the cylinder face, and adiabatic no-slip conditions are applied at the cylinder wall. The pressure is specified at the outlet boundary. For the simulations in this subsection, the governing equations, Eq. (1), are Favre-filtered and the
Vreman subgrid-scale model [60] is used as turbulence closure. It is reported that subgrid-scale models have little influence on the mean statistics for supercritical jets [7] and therefore no comparisons with different subgrid-scale models are conducted. The dynamic viscosity and thermal conductivity are evaluated following the models introduced in Section 3.2. The hybrid scheme with entropy stability is used and the RS-sensor is set to a value of $\zeta = 0.2$. The subgrid-scale model is only applied in the region where the non-dissipative high-order scheme is used to minimize the effects of numerical dissipation. The CFL-number is set to a value of 1.0 for all simulations.

Grid convergence studies are conducted for both cases using three different meshes. The mesh characteristics are shown in Table 3. The unstructured mesh is generated from a base hexahedral mesh and then adapted and refined in the region of interest. The minimum resolution of the mesh is in the region near the injector to resolve the large density gradients across the shear layer.

Figure 25 shows instantaneous results of simulations for Cases 3 and 4. Density iso-surfaces for values of 243 kg/m$^3$ and 108 kg/m$^3$ are shown for Case 3 and Case 4, respectively, and the temperature contours at the center-plane are also plotted. The density values are chosen to be the average of the injection and ambient densities. Figure 25 shows that the breakup length of the nitrogen jet in Case 3 is longer than that in Case 4. This can be attributed to the larger density
Table 3
Mesh resolution and size used in the grid convergence study of the cryogenic N₂ injection case.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Min mesh spacing [mm]</th>
<th>Mesh size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coarse</td>
<td>0.044</td>
<td>4.0 × 10⁶</td>
</tr>
<tr>
<td>Medium</td>
<td>0.031</td>
<td>8.2 × 10⁶</td>
</tr>
<tr>
<td>Fine</td>
<td>0.022</td>
<td>17.3 × 10⁶</td>
</tr>
</tbody>
</table>

Fig. 25. Instantaneous flow field in the cryogenic N₂ injection case for (a) Cases 3 and (b) Case 4. Density iso-surfaces with values equal to 243 kg/m³ and 108 kg/m³ for both cases are plotted on top of the temperature contours at the center-plane. Results from medium mesh are shown.

Fig. 26. Mean centerline density profiles of the cryogenic N₂ injection case in comparison with experimental data of Mayer et al. [59].
ratio between the injected and ambient nitrogen fluids. The simulation results are averaged over four flow-through-times to obtain statistics, and one flow-through-time corresponds to the time for the jet to convect 30d at the injection velocity. Figure 26 shows mean centerline density profiles using different meshes for both cases. As can be seen in Fig. 26, the results from the medium and fine meshes have almost identical mean density profile, demonstrating mesh convergence of the simulations. In comparison with experimental measurements from Mayer et al. [59], the simulation results obtained from the current study capture the behavior of the cryogenic nitrogen jet in the experiment. The present results show longer breakup length compared to those by Schmitt et al. [12] for both cases. This can be attributed to the omission of turbulence in the inflow conditions which is known to facilitate an earlier breakup of the nitrogen jet.

6. Conclusions

A finite-volume algorithm for simulating transcritical real-fluid mixing with large density gradients is presented. The spurious pressure oscillations that are present in transcritical simulations are due to large jumps in thermodynamic properties that arise from nonlinearities in the real-fluid EoS. Pressure oscillations are more severe than for ideal gas conditions and could cause the divergence of the simulation. A double-flux model is formulated for transcritical simulations by introducing an effective specific heat ratio based on the speed of sound to eliminate spurious pressure oscillations. A high-order non-dissipative hybrid scheme is used to address large density gradients while resolving the high-Reynolds number turbulent flow. An algorithm is designed to ensure the entropy-stable property of the numerical scheme through flux correction. The entropy-stable flux is shown to dampen numerical oscillations across the contact interface to ensure positivity of the mass fraction. A series of test cases is conducted at different operating conditions relevant to practical applications. No spurious pressure oscillations are observed for all test cases and numerical oscillations due to nonlinear instabilities are successfully dampened by the entropy-stable flux. Multiple test cases demonstrate the improved performance of the present numerical scheme over fully conservative schemes. The conservation errors generated by the double-flux formulation are acceptable and convergence with respect to mesh resolution is assessed. The multi-dimensional test cases show the performance of the developed numerical scheme for simulating transcritical flows in real applications.

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Appendix A. Thermodynamic relations based on Peng–Robinson state equation

A.1. Mixing rules

For mixtures, the coefficients a and b in Eq. (6) are evaluated as:

\[
a = \sum_{\alpha=1}^{N_S} \sum_{\beta=1}^{N_S} X_\alpha X_\beta a_{\alpha\beta},
\]

\[
b = \sum_{\alpha=1}^{N_S} X_\alpha b_\alpha,
\]

where \(X_\alpha\) is the molar fraction of species \(\alpha\). The coefficients \(a_{\alpha\beta}\) and \(b_\alpha\) are evaluated using the recommended mixing rules by Harstad et al. [61]:

\[
a_{\alpha\beta} = 0.457236 \frac{(RT_{c,\alpha\beta})^2}{p_{c,\alpha\beta}} \left(1 + c_{\alpha\beta} \left(1 - \frac{T}{T_{c,\alpha\beta}}\right)\right)^2,
\]

\[
b_\alpha = 0.077796 \frac{RT_{c,\alpha}}{p_{c,\alpha}},
\]

\[
c_{\alpha\beta} = 0.37464 + 1.54226 \omega_{\alpha\beta} - 0.26992 \omega_{\alpha\beta}^2.
\]

The critical mixture conditions for temperature, pressure, molar volume, compressibility, and acentric factor are determined using the corresponding state principles as:

\[
T_{c,\alpha\beta} = \sqrt{T_{c,\alpha} T_{c,\beta}(1 - k_{\alpha\beta})},
\]

\[
p_{c,\alpha\beta} = \frac{Z_{c,\alpha\beta}}{v_{c,\alpha\beta}} R T_{c,\alpha\beta},
\]
\[
\begin{align*}
\tau_{c,\alpha\beta} &= \frac{1}{8} \left( \frac{1}{3} + \frac{3}{3} \right)^3, \\
Z_{c,\alpha\beta} &= \frac{1}{2} (Z_{c,\alpha} + Z_{c,\beta}), \\
\omega_{\alpha\beta} &= \frac{1}{2} (\omega_{\alpha} + \omega_{\beta}),
\end{align*}
\]  

where \( R \) is the universal gas constant, \( T_c \) is the critical temperature, \( p_c \) is the critical pressure, \( \tau_c \) is the critical molar volume, \( Z_c \) is the critical compressibility factor, \( k_{\alpha\beta} \) is the binary interaction parameter, and \( \omega \) is the acentric factor.

A.2. Partial derivatives

Thermodynamic quantities in this study are evaluated consistently with the EoS and do not rely on tabulation or linearization methods. Partial derivatives and thermodynamic quantities based on PR-EoS, which are useful in the following for evaluating other thermodynamic variables, are listed below:

\[
\begin{align*}
\left( \frac{\partial p}{\partial T} \right)_{v,X_i} &= \frac{R}{v - b} - \frac{\partial (\alpha T) X_i}{\partial T} X_i, \\
\left( \frac{\partial p}{\partial v} \right)_{T,X_i} &= -\frac{RT}{v - b} \left\{ 1 - 2a \left[ RT^2 \left( \frac{v^2 + 2bv - b^2}{v^2 - b^2} \right) \right]^{-1} \right\}, \\
\left( \frac{\partial a}{\partial T} \right)_{X_i} &= -\frac{1}{T} \sum_{\alpha=1}^{N_1} \sum_{\beta=1}^{N_2} X_{\alpha} X_{\beta} a_{\alpha\beta} G_{\alpha\beta}, \\
\left( \frac{\partial^2 a}{\partial T^2} \right)_{X_i} &= 0.457236 \frac{R^2}{2T} \sum_{\alpha=1}^{N_1} \sum_{\beta=1}^{N_2} X_{\alpha} X_{\beta} c_{\alpha\beta} (1 + c_{\alpha\beta}) \frac{T_{c,\alpha\beta}}{p_{c,\alpha\beta}} \frac{1}{T} - \frac{T_{c,\alpha\beta}}{T}, \\
G_{\alpha\beta} &= \frac{c_{\alpha\beta} \sqrt{T_c}}{1 + c_{\alpha\beta} (1 - \sqrt{T_c})}, \\
K_1 &= \int_{+\infty}^{v} \frac{1}{v^2 + 2bv - b^2} dv = \frac{1}{2\sqrt{2}b} \ln \left( \frac{v + (1 - \sqrt{2})b}{v + (1 + \sqrt{2})b} \right).
\end{align*}
\]

A.3. Internal energy, enthalpy and entropy

For general real fluids, thermodynamic quantities are typically evaluated from the ideal-gas value and a departure function, which accounts for the deviation from the ideal-gas behavior. The ideal-gas enthalpy, entropy and specific heat can be evaluated from NASA polynomials at a reference temperature of 298 K. In the following, superscript zero indicates the ideal-gas value of the thermodynamic quantity. The simple mixture-averaged mixing rule is used for ideal-gas mixtures.

The specific internal energy can be written as,

\[
e(T, \rho, X_i) = e^0(T, X_i) + \int_0^\rho \left[ p - T \left( \frac{\partial p}{\partial T} \right)_{\rho,X_i} \right] \frac{d\rho}{\rho^2},
\]

and can be integrated analytically for a specific EoS (here, PR-EoS):

\[
e = e^0 + K_1 \left[ a - T \left( \frac{\partial a}{\partial T} \right)_{X_i} \right].
\]

The specific enthalpy can be evaluated from \( h = e + pv \), and we have

\[
h = h^0 - RT + K_1 \left[ a - T \left( \frac{\partial a}{\partial T} \right)_{X_i} \right] + pv.
\]

The specific entropy can be expressed as a combination of ideal-gas value and departure function,
\[ s(T, \rho, X_i) = s^0(T, \rho, X_i) + \int_0^\rho \left[ \rho R - \left( \frac{\partial p}{\partial T} \right)_{\rho, X_i} \right] \frac{d\rho}{\rho^2}, \]
\[(41)\]
and integrated as,
\[ s = s^0 + R \ln \frac{v - b}{v} - K_1 \left( \frac{\partial a}{\partial T} \right)_{X_i}. \]
\[(42)\]
Partial enthalpies for each species, \( h_k \), can be evaluated using the partial derivatives with respect to mole fractions. The procedures to evaluate the partial enthalpy for real-fluids are similar to those in [62] and therefore omitted here.

A.4. Specific heat capacity

The specific heat capacity at constant volume is evaluated as
\[ c_v = \left( \frac{\partial e}{\partial T} \right)_{v, X_i} = c_v^0 - K_1 T \left( \frac{\partial^2 a}{\partial T^2} \right)_{X_i}, \]
\[(43)\]
where \( c_v^0 \) is the specific heat at constant volume for ideal gas. The specific heat capacity at constant pressure is evaluated as
\[ c_p = \left( \frac{\partial h}{\partial T} \right)_{p, X_i} = c_p^0 - R - K_1 T \left( \frac{\partial^2 a}{\partial T^2} \right)_{X_i} - T \frac{\left( \frac{\partial p}{\partial T} \right)^2}{\left( \frac{\partial p}{\partial v} \right)_{T, X_i}}, \]
\[(44)\]
where \( c_p^0 \) is the specific heat at constant pressure for ideal gas, and the last term is the difference between the two specific heat capacities [43].

A.5. Speed of sound

The speed of sound for general real-fluids can be evaluated as
\[ c^2 = \left( \frac{\partial p}{\partial \rho} \right)_{s, X_i} = \frac{\gamma}{\rho \kappa_T}, \]
\[(45)\]
where \( \gamma \) is the specific heat ratio and \( \kappa_T \) is the isothermal compressibility, which is defined as
\[ \kappa_T = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial p} \right)_{T, X_i}. \]
\[(46)\]

Appendix B. Hyperbolicity of Euler system with cubic equation of state

For a complete EoS, \( e = e(v, s) \), the thermodynamic stability requires that \( e \) be jointly convex as a function of \( v \) and \( s \), so that the Hessian matrix should be positive semidefinite [19,63–65]
\[ \left( \frac{\partial^2 e}{\partial s^2} \right)_v \geq 0, \quad \left( \frac{\partial^2 e}{\partial v^2} \right)_s \geq 0, \quad \left( \frac{\partial^2 e}{\partial s \partial v} \right)_v \left( \frac{\partial^2 e}{\partial v \partial s} \right)_v \geq \left( \frac{\partial^2 e}{\partial s \partial v} \right)_v^2, \]
\[(47)\]
which translates into the requirements
\[ c_v^{-1} \geq c_p^{-1} \geq 0, \quad \kappa_s^{-1} \geq \kappa_T^{-1} \geq 0, \]
\[(48)\]
where \( \kappa_s \) is the isentropic compressibility. One of the requirements, \( (\partial^2 e/\partial v^2)_s \geq 0 \), implies a real-valued speed of sound, which is a necessary condition for the convexity of an EoS.

The hyperbolicity of the Euler system does not rely on the EoS used, as long as the speed of sound is real. For cubic EoS, this is always true outside the vapor dome, as shown in Fig. 27. Inside the vapor dome, the thermodynamic state described by the EoS is either metastable or unstable/non-convex. In Fig. 27, the unstable/non-convex region is enclosed by the spinodal curves which are the loci of \( (\partial p/\partial v)_T = 0 \). However, the speed of sound is real in a much larger region inside the vapor dome since the convexity of an EoS is a stronger condition than a real speed of sound as can be seen from Fig. 27.

Analysis of simulation results for test cases, presented in Section 5, show that solution are within the hyperbolic region of the corresponding Euler system with a real-valued speed of sound. However, in the two-dimensional nitrogen injection case discussed in Section 5.4, a small fraction of the solutions may occupy the unstable region of the PR EoS due to the larger pressure fluctuations caused by the two-dimensionality and confined domain, as can be seen in Fig. 28(a). This is not seen in the three-dimensional nitrogen injection case as shown in Fig. 28(b), or all other test cases in this study.
Appendix C. Evaluation of temperature from density, pressure and species

In the following, procedures to obtain temperature given density, pressure and species for PR-EoS are outlined. A similar procedure can be formulated for other cubic state equations. From Eqs. (6), (34), (35), a quadratic equation for \( \Theta = \sqrt{T} \) can be obtained after some algebra:

\[
C_1 \Theta^2 + C_2 \Theta + C_3 = 0, \tag{49}
\]

where

\[
C_1 = \frac{R}{v - b} - \frac{1}{v^2 + 2bv - b^2} \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} 0.457236 X_{\alpha} X_{\beta} \frac{(RT_{c,\alpha\beta})^2}{p_{c,\alpha\beta}} \frac{c_{\alpha\beta}^2}{T_{c,\alpha\beta}}, \tag{50a}
\]

\[
C_2 = \frac{1}{v^2 + 2bv - b^2} \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} 0.457236 X_{\alpha} X_{\beta} \frac{(RT_{c,\alpha\beta})^2}{p_{c,\alpha\beta}} \frac{2(c_{\alpha\beta} + c_{\alpha\beta}^2)}{\sqrt{T_{c,\alpha\beta}}}, \tag{50b}
\]

\[
C_3 = -p - \frac{1}{v^2 + 2bv - b^2} \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} 0.457236 X_{\alpha} X_{\beta} \frac{(RT_{c,\alpha\beta})^2}{p_{c,\alpha\beta}} (1 + 2c_{\alpha\beta} + c_{\alpha\beta}^2). \tag{50c}
\]

The square root of temperature can be solved analytically from the roots of the quadratic equations and the positive root is taken as the solution to obtain the temperature.
Appendix D. 1D MATLAB code for the double-flux model

A one-dimensional version of the double-flux model is provided in MATLAB code for the readers as supplementary materials available at https://github.com/IhmeGroup/DoubleFlux-1D. A first-order upwinding scheme is used for the brevity of the code. Thermodynamic quantities are obtained through the PR EoS. The double-flux model is implemented following Algorithm 1. Detailed comments are provided within each function with corresponding equations denoted for the readers. The code can also be downloaded from: http://dx.doi.org/10.1016/j.jcp.2017.03.022.

References


