# Extension of the entropy viscosity method to the multi-D 7-equation two-phase flow model.

### I do not know if we should have 'multi-D' in the title since we will only present 1-D results

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#### Abstract

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Key words: two-phase flow model, with variable area, entropy viscosity method, stabilization method, low Mach regime, shocks.

#### 1 1. Introduction

- a few lines about the need for accurately resolving two-phase flows
- background on the different two-phase flow models: 5, 6 and 7-equation two-phase flow models
- then, focus on the different types of 7-equation two-phase flow models: they mostly differ because of the closure relaxations used
- discuss the different numerical solvers developed for the 7-equation twophase flow model: HLL, HLLC, and approximated Riemann solvers accounting for the source terms
- emphasize the fact that the above numerical solvers only works on discontinuous schemes
- then, introduce the entropy viscosity method and details the organization of the paper

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Compressible two-phase flows are found in numerous industrial applications and are an ongoing area of research in modeling and simulation over many years. A variety of models with different levels of complexity has been developed such 16 as: five-equation model [1], six-equation model [2], and more recently the sevenequation model [3]. These models are all obtained by integrating the single-18 phase flow balance equations weighed by a characteristic or indicator function 19 for each phase. The resulting system of equations contains non-conservative 20 terms that describe the interaction between phases but also an equation for the 21 volume fraction. Once a system of equations describing the physics is derived, 22 the next challenging step is to develop a robust and accurate discretization to obtain a numerical solution. Assuming that the system of equations is hyper-24 bolic under some conditions, a Riemann solver could be used but is often ruled 25 out because of the complexity due to the number of equations involved. Further-26 more, careless approximation for the treatment of the non-conservative terms 27 can lead to failure in computing the numerical solution [4]. An alternative is to use an approximate Riemann solver, a well-established approach for single-phase 29 flows, while deriving a consistent discretization scheme for the non-conservative 30 31

This methodology was applied to the seven-equation model (SEM) introduced by Berry et al. in [3]. This model is known to be unconditionally hyperbolic which is highly desirable when working with approximate Riemann solvers and can treat a wide range of applications. Its particularity comes from the pressure and velocity relaxation terms in the volume fraction, momentum and energy equations that can bring the two phases in equilibrium when using large values of the relaxation parameters. In other words, the seven-equation model can degenerate into the six- and five-equation models. Alike for the other twophase flow models, solving for the seven-equation model requires a numerical solver and significant effort was dedicated to this task for spatially discontinuous schemes. Because each phase is assumed to obey the Euler equations, most of the numerical solvers are adapted from the single-phase approximate Riemann solvers. For example, Saurel et al. [5, 6] employed a HLL-type scheme to solve for the SEM but noted that excessive dissipation was added to the contact discontinuity. A more advanced HLLC-type scheme was developed in [7] but only for the subsonic case and then extended to supersonic flows in [8]. More recently, Ambroso et al. [9] proposed an approximate Riemann solver accounting for source terms such as gravity and drag forces, but with no interphase mass transfer.

#### 51 2. The multi-D 7-equation two-phase flow model

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The multi-D seven-equation two-phase model presented in this paper is obtained by assuming that each phase obeys the single-phase Euler equations (with phase-exchange terms) and by integrating over a control volume after multiplying by a characteristic function. The detailed derivation can be found in [3]. In this section, the governing multi-dimensional equations are recalled for a phase k in interaction with a phase j. Each phase obeys the following mass,

momentum and energy balance equations, supplemented by a non-conservative volume-fraction equation:

$$\frac{\partial (\alpha \rho)_k A}{\partial t} + \nabla \cdot (\alpha \rho \boldsymbol{u} A)_k = -\Gamma A_{int} A \tag{1a}$$

$$\frac{\partial (\alpha \rho \boldsymbol{u})_k A}{\partial t} + \boldsymbol{\nabla} \cdot [\alpha_k A (\rho \boldsymbol{u} \otimes \boldsymbol{u} + P \mathbb{I})_k] = P_{int} A \boldsymbol{\nabla} \alpha_k + P_k \alpha_k \boldsymbol{\nabla} A + A \lambda_u (\boldsymbol{u}_i - \boldsymbol{u}_k) - \Gamma A_{int} \boldsymbol{u}_{int} A \quad (1b)$$

$$\frac{\partial (\alpha \rho E)_k A}{\partial t} + \nabla \cdot [\alpha_k \mathbf{u}_k A (\rho E + P)_k] = P_{int} \mathbf{u}_{int} A \nabla \alpha_k - \bar{P}_{int} A \mu_P (P_k - P_j) 
+ \bar{\mathbf{u}}_{int} A \lambda_u (\mathbf{u}_j - \mathbf{u}_k) + \Gamma A_{int} \left( \frac{P_{int}}{\rho_{int}} - H_{k,int} \right) A$$
(1c)

$$\frac{\partial \alpha_k A}{\partial t} + A \boldsymbol{u}_{int} \cdot \boldsymbol{\nabla} \alpha_k = A \mu_P (P_k - P_j) - \frac{\Gamma A_{int} A}{\rho_{int}}$$
 (1d)

where  $\alpha_k$ ,  $\rho_k$ ,  $\boldsymbol{u}_k$  and  $E_k$  denote the volume fraction, the density, the velocity vector and the total specific energy of phase k, respectively. The phase pressure  $P_k$  is computed from an equation of state. The interfacial pressure and velocity and their corresponding average values are denoted by  $P_{int}$ ,  $\boldsymbol{u}_{int}$ ,  $\bar{P}_{int}$  and  $\bar{\boldsymbol{u}}_{int}$ , respectively, and are defined in Eq. (2).

$$P_{int} = \bar{P}_{int} + \frac{Z_k Z_j}{Z_k + Z_j} \frac{\nabla \alpha_k}{||\nabla \alpha_k||} \cdot (\boldsymbol{u}_j - \boldsymbol{u}_k)$$
 (2a)

$$\bar{P}_{int} = \frac{Z_j P_k + Z_k P_j}{Z_k + Z_j} \tag{2b}$$

$$\mathbf{u}_{int} = \bar{\mathbf{u}}_{int} + \frac{\nabla \alpha_k}{||\nabla \alpha_k||} \frac{P_j - P_k}{Z_k + Z_j}$$
 (2c)

$$\bar{\boldsymbol{u}}_{int} = \frac{Z_k \boldsymbol{u}_k + Z_j \boldsymbol{u}_j}{Z_k + Z_j}.$$
 (2d)

The interfacial specific total enthalpy of phase k,  $H_k$ , is defined as follows:  $H_k = h_k + 0.5||\mathbf{u}||^2$ . Following [3], the pressure and velocity relaxation coefficients,  $\mu_P$  and  $\lambda_u$  respectively, are function of the acoustic impedance  $Z_k = \rho_k c_k$  and the specific interfacial area  $A_{int}$  as shown in Eq. (3).

$$\lambda_u = \frac{1}{2} \mu_P Z_k Z_j \tag{3a}$$

$$\mu_P = \frac{A_{int}}{Z_k + Z_j} \tag{3b}$$

The specific interfacial area (i.e., the interfacial surface area per unit volume of two-phase mixture),  $A_{int}$ , must be specified from some type of flow regime

map or function under the form of a correlation. In [3],  $A_{int}$  is chosen to be a function of the liquid volume fraction:

$$A_{int} = A_{int}^{max} \left[ 6.75 \left( 1 - \alpha_k \right)^2 \alpha_k \right], \tag{4}$$

where  $A_{int}^{max} = 5100 \ m^2/m^3$ . With such definition, the interfacial area is zero in the limits  $\alpha_k = 0$  and  $\alpha_k = 1$ . Lastly,  $\Gamma$  is the net mass transfer rate per unit interfacial area from phase j to phase k. Its expression, given in Eq. (5), is obtained by considering a vaporization/condensation process that is dominated by heat diffusion at the interface [3, 10]:

$$\Gamma = \Gamma_{j} = \frac{h_{T,k} (T_{k} - T_{int}) + h_{T,j} (T_{j} - T_{int})}{h_{j,int} - h_{k,int}}$$

$$= \frac{h_{T,k} (T_{k} - T_{int}) + h_{T,j} (T_{j} - T_{int})}{L_{v} (T_{int})},$$
(5)

where  $L_v(T_{int}) = h_{j,int} - h_{k,int}$  represents the latent heat of vaporization. The interface temperature is determined by the saturation constraint  $T_{int} = T_{sat}(P)$  with the appropriate pressure  $P = \bar{P}_{int}$  determined above. The interfacial heat transfer coefficients for phases k and j are denoted by  $h_{T,k}$  and  $h_{T,j}$ , respectively, and computed from correlations [3].

The set of equations obeyed by phase j are simply obtained by substituting k by j and j by k in Eq. (1), keeping the same definition of the interfacial variables and remembering that  $\Gamma_j = -\Gamma_k$ . In the case of two-phase flows, the equation for the volume fraction of phase j is simply replaced by the algebraic relation

$$\alpha_i = 1 - \alpha_k$$

which reduces the number of equations from eight to seven and yields the sevenequation two-phase flow model.

The seven-equation model has interesting properties that are discussed next. A set of seven waves is present in such a model: two acoustic waves and a contact wave for each phase supplanted by a volume fraction wave propagating at the interfacial velocity  $u_{int}$ . Considering a domain of dimension  $\mathbb{D}$ , the corresponding eigenvalues are the following for each phase k:

$$\lambda_{1} = \mathbf{u}_{int} \cdot \bar{\mathbf{n}}$$

$$\lambda_{2,k} = \mathbf{u}_{k} \cdot \bar{\mathbf{n}} - c_{k}$$

$$\lambda_{3,k} = \mathbf{u}_{k} \cdot \bar{\mathbf{n}} + c_{k}$$

$$\lambda_{d+3,k} = \mathbf{u}_{k} \cdot \bar{\mathbf{n}} \text{ for } d = 1 \dots \mathbb{D},$$
(6)

where  $\bar{n}$  is an unit vector pointing to a given direction. The eigenvalues given in Eq. (6) are unconditionally real which presents an interesting property for the development of numerical methods since the system is hyperbolic and well-posed. To relax the seven-equation model to the ill-posed classical six-equation

model, only the pressures should be relaxed toward a single pressure for both phases. This is accomplished by specifying the pressure relaxation coefficient to be very large, i.e., letting it approach infinity. But if the pressure relaxation coefficient goes to infinity, so does the velocity relaxation rate also approach infinity. This then relaxes the seven-equation model not to the classical sixequation model but to the mechanical equilibrium five-equation model of Kapila [1]. This reduced five-equation model is also hyperbolic and well-posed. The five-equation model provides a very useful starting point for constructing multidimensional interface resolving methods which dynamically captures evolving and spontaneously generated interfaces [11]. Thus the seven-equation model can be relaxed locally to couple seamlessly with such a multi-dimensional, interface resolving code. Numerically, the mechanical relaxation coefficients  $\mu_P$ (pressure) and  $\lambda_u$  (velocity) can be relaxed independently to yield solutions to useful, reduced models. It is noted, however, that relaxation of pressure only by making  $\mu_P$  large without relaxing velocity will indeed give ill-posed and unstable numerical solutions, just as the classical six-equation two-phase model does, with sufficiently fine spatial resolution, as confirmed in [3, 12]. For each phase k, an entropy equation can be derived when accounting only for the pressure and velocity relaxation terms (all of the terms proportional to the net mass transfer term  $\Gamma$  are removed). The entropy function for a phase k is denoted by  $s_k$  and function of the density  $\rho_k$  and the internal energy  $e_k$ . The derivation is detailed in Appendix A and only the final result is recalled here:

$$(s_e)_k^{-1} \alpha_k \rho_k A \frac{Ds_k}{Dt} = \mu_P \frac{Z_k}{Z_k + Z_j} (P_j - P_k)^2 + \lambda_u \frac{Z_j}{Z_k + Z_j} (\boldsymbol{u}_j - \boldsymbol{u}_k)^2$$
$$\frac{Z_k}{(Z_k + Z_j)^2} \left[ Z_j (\boldsymbol{u}_j - \boldsymbol{u}_k) + \frac{\boldsymbol{\nabla} \alpha_k}{||\boldsymbol{\nabla} \alpha_k||} (P_k - P_j) \right]^2. \tag{7}$$

The partial derivative of the entropy function  $s_k$  with respect to the internal energy  $e_k$ ,  $(s_e)_k$ , is shown to be proportional to the inverse of the temperature of phase k, alike for the single phase Euler equations [13, 14]. The right hand-side of Eq. (7) is unconditionally positive since all terms are squared and thus, is used to demonstrate the entropy minimum principle and derive the dissipative terms. Furthermore, Eq. (7) is valid for both phases  $\{k, j\}$  and ensures positivity of the total entropy equation that is obtained by summing over the phases:

$$\sum_{k} (s_e)_k^{-1} \alpha_k \rho_k A \frac{Ds_k}{Dt} = \sum_{k} (s_e)_k^{-1} \alpha_k \rho_k A \left( \partial_t s_k + \boldsymbol{u}_k \cdot \boldsymbol{\nabla} s_k \right) \ge 0.$$
 (8)

Note that when one phase disappears, Eq. (8) degenerates into the single phase entropy equation [3, 14].

## 3. A viscous regularization for the multi-D seven-equation two-phase flow model

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We now propose to derive a viscous regularization for the seven-equation model given in Eq. (1) by using the same methodology as for the multi-D Euler

equations with/without variable area [13, 15]. The method consists in adding perturbation terms to the system of equation under consideration, and re-derive 77 the entropy equation whose sign is known to be positive to ensure uniqueness 78 of the numerical solution [16]. Because of the addition of perturbation terms, 79 the entropy equation is modified and contains extra terms of unknown sign. 80 By carefully choosing a definition for each of the perturbation term, the sign 81 of the entropy equation can be determined and proved positive. For the seven-82 equation model, derivation of a viscous regularization can be achieved by consid-83 ering either the phasic entropy equation (Eq. (7)) or the total entropy equation 84 (Eq. (8)). In the later case, the entropy minimum principle is verified for the whole system which may not ensure positivity of the entropy equation for each phase. However, positivity of the total entropy equation can be also achieved 87 by assuming that the entropy minimum principle holds for each phase. This 88 stronger requirement will also ensure consistency with the single phase Euler 89 equations when one of the phase disappears in the limits  $\alpha_k \to 0$  and  $\alpha_k \to 1$ . Thus, it is chosen to work with the phasic entropy equations. 91

For the purpose of this section, the system of equations given in Eq. (9) is considered which is obtained by simply omitting the mass source terms (terms proportional to  $\Gamma$ ) in Eq. (1).

$$\partial_t \left( \alpha_k A \right) + A \boldsymbol{u}_{int} \cdot \boldsymbol{\nabla} \alpha_k = A \mu_P \left( P_k - P_i \right) \tag{9a}$$

$$\partial_t \left( \alpha_k \rho_k A \right) + \nabla \cdot \left( \alpha_k \rho_k \boldsymbol{u}_k A \right) = 0 \tag{9b}$$

$$\partial_{t} \left( \alpha_{k} \rho_{k} u_{k} A \right) + \nabla \cdot \left[ \alpha_{k} A \left( \rho_{k} \boldsymbol{u}_{k} \otimes \boldsymbol{u}_{k} + P_{k} \mathbb{I} \right) \right] = \alpha_{k} P_{k} \nabla A + P_{int} A \nabla \alpha_{k} + A \lambda_{u} \left( \boldsymbol{u}_{j} - \boldsymbol{u}_{k} \right)$$
(9c)

$$\partial_{t} \left( \alpha_{k} \rho_{k} E_{k} A \right) + \nabla \cdot \left[ \alpha_{k} A \boldsymbol{u}_{k} \left( \rho_{k} E_{k} + P_{k} \right) \right] = A P_{int} \boldsymbol{u}_{int} \cdot \nabla \alpha_{k} - \mu_{P} \bar{P}_{int} \left( P_{k} - P_{j} \right) + A \lambda_{u} \bar{\boldsymbol{u}}_{int} \cdot \left( \boldsymbol{u}_{j} - \boldsymbol{u}_{k} \right)$$
(9d)

In order to apply the entropy viscosity method, perturbation terms are added to each equation of Eq. (9), which yields:

$$\partial_t (\alpha_k A) + \boldsymbol{u}_{int} A \boldsymbol{\nabla} \alpha_k = A \mu_P (P_k - P_i) + \boldsymbol{\nabla} \cdot \boldsymbol{l}_k \tag{10a}$$

$$\partial_t \left( \alpha_k \rho_k A \right) + \nabla \cdot \left( \alpha_k \rho_k \boldsymbol{u}_k A \right) = \nabla \cdot \boldsymbol{f}_k \tag{10b}$$

$$\partial_{t} (\alpha_{k} \rho_{k} \boldsymbol{u}_{k} A) + \boldsymbol{\nabla} \cdot [\alpha_{k} A (\rho_{k} \boldsymbol{u}_{k} \otimes \boldsymbol{u}_{k} + P_{k} \mathbb{I})] = \alpha_{k} P_{k} \boldsymbol{\nabla} A + P_{int} A \boldsymbol{\nabla} \alpha_{k} + A \lambda_{u} (\boldsymbol{u}_{j} - \boldsymbol{u}_{k}) + \boldsymbol{\nabla} \cdot \boldsymbol{g}_{k} \quad (10c)$$

$$\partial_{t} (\alpha_{k} \rho_{k} E_{k} A) + \nabla \cdot [\alpha_{k} A \boldsymbol{u}_{k} (\rho_{k} E_{k} + P_{k})] = P_{int} A \boldsymbol{u}_{int} \cdot \nabla \alpha_{k} - \mu_{P} \bar{P}_{int} (P_{k} - P_{j}) + A \lambda_{u} \bar{\boldsymbol{u}}_{int} \cdot (\boldsymbol{u}_{j} - \boldsymbol{u}_{k}) + \nabla \cdot (\boldsymbol{h}_{k} + \boldsymbol{u} \cdot \boldsymbol{g}_{k})$$

$$(10d)$$

where  $f_k$ ,  $g_k$ ,  $h_k$  and  $l_k$  are the phasic perturbation terms. The next step consists in deriving the entropy equation for the phase k, on the same model as what is done in Appendix A for the system of equations (Eq. (9)) that does not contain the perturbation terms.

1. derive the density and internal energy equations from Eq. (10).

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102 103 2. assuming that the phasic entropy,  $s_k$ , is function of the density,  $\rho_k$  and the internal energy,  $e_k$ , derive the entropy equation by using the chain rule:

$$\frac{Ds_k}{Dt} = (s_\rho)_k \frac{D\rho_k}{Dt} + (s_e)_k \frac{De_k}{Dt}$$
(11)

where  $\frac{D}{Dt}$  is the material derivative. The terms  $(s_e)_k$  and  $(s_\rho)_k$  denote the partial derivative of the entropy  $s_k$  with respect to  $e_k$  and  $\rho_k$ , respectively.

3. isolate the terms of interest and choose an appropriate expression for each of the perturbation terms in order to ensure positivity of the right-hand side.

We first derive the density equation for the primitive variable  $\rho_k$  by combining Eq. (10a) and Eq. (10b) to obtain:

$$\alpha_k A \left[ \partial_t \rho_k + \left( \boldsymbol{u}_k - \underline{\boldsymbol{u}}_{int} \right) \cdot \boldsymbol{\nabla} \rho_k \right] = \underline{A \rho_k \mu_P \left( P_k - P_j \right)} + \boldsymbol{\nabla} \cdot \boldsymbol{f}_k - \rho_k \boldsymbol{\nabla} \cdot \boldsymbol{l}_k \quad (12)$$

In order to derive the internal energy equation, the velocity equation is obtained by subtracting the density equation from the momentum equation:

$$\alpha_{k}\rho_{k}A\left[\partial_{t}\boldsymbol{u}_{k}+\boldsymbol{u}_{k}\cdot\boldsymbol{\nabla}\cdot\boldsymbol{u}_{k}\right]+\boldsymbol{\nabla}\cdot\left(\alpha_{k}\rho_{k}AP_{k}\mathbb{I}\right)=$$

$$\alpha_{k}P_{k}\boldsymbol{\nabla}A+P_{int}A\boldsymbol{\nabla}\alpha_{k}+A\lambda\left(\boldsymbol{u}_{j}-\boldsymbol{u}_{k}\right)+\boldsymbol{\nabla}\cdot\boldsymbol{g}_{k}-\boldsymbol{u}_{k}\otimes\boldsymbol{f}_{k}$$
(13)

After multiplying Eq. (13) by the velocity vector  $\mathbf{u}_k$ , the resulting kinetic energy equation is subtracted from the total energy equation to obtain the internal energy equation for phase k:

$$\alpha_{k}\rho_{k}A\left[\partial_{t}\boldsymbol{e}_{k}+\boldsymbol{u}_{k}\cdot\boldsymbol{\nabla}\cdot\boldsymbol{e}_{k}\right]+\alpha_{k}\rho_{k}AP_{k}\boldsymbol{\nabla}\boldsymbol{u}_{k}=\underbrace{\frac{P_{int}A\left(\boldsymbol{u}_{int}-\boldsymbol{u}_{k}\right)\cdot\boldsymbol{\nabla}\alpha_{k}}{-\bar{P}_{int}A\mu_{P}\left(P_{k}-P_{j}\right)}}_{+\boldsymbol{\nabla}\cdot\boldsymbol{h}_{k}+\boldsymbol{g}_{k}:\boldsymbol{\nabla}\boldsymbol{u}_{k}}-\underbrace{\frac{\alpha_{k}P_{k}\boldsymbol{u}_{k}\boldsymbol{\nabla}A}{-\underline{\alpha_{k}P_{k}\boldsymbol{u}_{k}\boldsymbol{\nabla}A}}}_{|\boldsymbol{u}_{j}-\boldsymbol{u}_{k}\rangle\cdot(\bar{\boldsymbol{u}}_{int}-\boldsymbol{u}_{k})}_{(14)}$$

The underline terms in Eq. (12) and Eq. (14) yield the positive terms in the right-hand-side of Eq. (7) and thus are ignored in the remaining of the derivation for simplicity. The entropy equation is now obtained by combining the density equation (Eq. (12)) and the internal energy equation (Eq. (14)) through the chain rule given in Eq. (11) to yield:

$$\alpha_{k}\rho_{k}A\frac{Ds_{k}}{Dt} = (\rho s_{\rho})_{k} \left[ \nabla \cdot \boldsymbol{f}_{k} - \rho_{k} \nabla \cdot \boldsymbol{l}_{k} \right] + (s_{e})_{k} \left[ \nabla \cdot \boldsymbol{h}_{k} + \boldsymbol{g}_{k} : \nabla \boldsymbol{u}_{k} + \left( ||\boldsymbol{u}||_{k}^{2} - e_{k} \right) \nabla \cdot \boldsymbol{f}_{k} \right],$$
(15)

where it was assumed that the entropy of phase k satisfies the second thermodynamic law:

$$T_k ds_k = de_k - P_k \frac{d\rho_k}{\rho_k^2}$$
which implies  $P_k(s_e)_k + \rho_k(s_\rho)_k = 0$ , (16)
$$(s_e)_k = T_k^{-1} \text{ and } (s_\rho)_k = -(s_e)_k P_k \frac{d\rho_k}{\rho_k^2}.$$

Eq. (16) is also used to compute the partial derivative of the entropy with respect to the density,  $(s_{\rho})_k$ , and the internal energy,  $(s_e)_k$ , if needed.

Following the methodology applied in [13, 15], the right-hand side of Eq. (15) can be further simplified by using the following expression for the dissipative terms  $f_k$ ,  $g_k$  and  $h_k$ :

$$\boldsymbol{f}_k = \tilde{\boldsymbol{f}}_k + \rho_k \boldsymbol{l}_k \tag{17a}$$

$$\boldsymbol{g}_k = \alpha_k \rho_k A \mu_k \mathbb{F}(\boldsymbol{u}_k) + \boldsymbol{f}_k \otimes \boldsymbol{u}_k \tag{17b}$$

$$\boldsymbol{h}_k = \tilde{\boldsymbol{h}}_k - \frac{||\boldsymbol{u}||^2}{2} \boldsymbol{f}_k + (\rho e)_k \boldsymbol{l}_k, \tag{17c}$$

where  $\mu_k$  is a positive viscosity coefficient for phase k. Note the area function A in the definition of g. Substituting the expression of the dissipative term given in Eq. (17) into Eq. (15), it yields:

$$\alpha_{k}\rho_{k}A\frac{Ds_{k}}{Dt} = \underbrace{\left(s_{e}\right)_{k}\alpha_{k}\rho_{k}A\mu_{k}\mathbb{F}(\boldsymbol{u}_{k}):\boldsymbol{\nabla}\boldsymbol{u}_{k}}_{\mathcal{R}_{1}} + \underbrace{\left[\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{h}}_{k} - e_{k}\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{f}}_{k}\right] + (\rho s_{\rho})_{k}\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{f}}_{k}}_{\mathcal{R}_{2}} + \underbrace{\left(s_{e}\right)_{k}\boldsymbol{\nabla}\cdot(\rho_{k}e_{k}\boldsymbol{l}_{k}) - (s_{e})_{k}e_{k}\boldsymbol{\nabla}\cdot(\rho_{k}\boldsymbol{l}_{k}) + \rho_{k}(s_{\rho})_{k}\boldsymbol{\nabla}\cdot(\rho_{k}\boldsymbol{l}_{k}) - \rho_{k}^{2}(s_{\rho})_{k}\boldsymbol{\nabla}\cdot\boldsymbol{l}_{k}}_{\mathcal{R}_{3}}.$$
(18)

We now split the right-hand-side of Eq. (18) into three residuals denoted by  $\mathcal{R}_1$ ,  $\mathcal{R}_2$  and  $\mathcal{R}_3$  and will study the sign of each of them. Since  $(s_e)_k$  is defined as the inverse of the temperature and thus positive, the sign of the first term,  $\mathcal{R}_1$ , is conditioned by the choice of the function  $\mathbb{F}(\boldsymbol{u}_k)$  so that the product with the tensor  $\nabla \boldsymbol{u}_k$  is positive. As in [13, 15],  $\mathbb{F}(\boldsymbol{u}_k)$  is chosen proportional to the symmetric gradient of the velocity vector  $\nabla^s \boldsymbol{u}_k$ , whom entries are given by  $((\nabla^s \boldsymbol{u})_{i,j})_k = \frac{1}{2} (\partial_{x_i} u_i + \partial_{x_j} u_j)_k$ . After a few lines of algebra, the third term  $\mathcal{R}_3$  can be recast as a function of the gradient of the entropy as follows:

$$\mathcal{R}_2 = \rho_k A \boldsymbol{l}_k \cdot \boldsymbol{\nabla} s_k. \tag{19}$$

One of the assumptions made in the entropy minimum principle is to that the entropy is at a minimum which implies that its gradient is null. Because of this, it follows that the term  $\mathcal{R}_3$  is zero at the minimum and thus, the entropy

minimum principle is verified independently of the definition of the perturbation term  $l_k$  used in the volume fraction equation Eq. (10a). It will be explained later in this section how to derive a definition for  $l_k$ .

We now focus on the term denoted by  $\mathcal{R}_2$ , that is found identical to the right-hand-side of the single phase entropy equation obtained from the multi-D Euler equations (see [13, 15]. Thus, the term  $\mathcal{R}_2$  is known to be positive when (i) assuming concavity of the entropy function  $s_k$  with respect to the internal energy  $e_k$  and the specific volume  $1/\rho_k$  (or convexity of  $-s_k$ ) and (ii) choosing the following definitions for the dissipative terms  $\tilde{h}_k$  and  $\tilde{f}_k$ :

$$\tilde{\boldsymbol{f}}_k = \alpha_k A \kappa_k \boldsymbol{\nabla} \rho_k \tag{20a}$$

$$\tilde{\boldsymbol{h}}_k = \alpha_k A \kappa_k \boldsymbol{\nabla} \left( \rho e \right)_k, \tag{20b}$$

where  $\kappa_k$  is another positive viscosity coefficient. The entropy equation can now be written in its final form:

$$\alpha_k \rho_k A \frac{Ds_k}{Dt} = \boldsymbol{f}_k \cdot \boldsymbol{\nabla} s_k + \boldsymbol{\nabla} \cdot (\alpha_k \rho_k A \boldsymbol{\nabla} s_k) - \alpha_k A \kappa_k \mathbf{Q}_k + (s_e)_k \alpha_k A \rho_k \mu_k \boldsymbol{\nabla}^s \boldsymbol{u}_k : \boldsymbol{\nabla} \boldsymbol{u}_k,$$
 (21)

where  $\mathbf{Q}_k$  is a negative semi-definite quadratic form defined as:

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$$\begin{aligned} \mathbf{Q}_k &= X_k^t \Sigma_k X_k \\ \text{with } X_k &= \begin{bmatrix} \boldsymbol{\nabla} \rho_k \\ \boldsymbol{\nabla} e_k \end{bmatrix} \text{ and } \Sigma_k = \begin{bmatrix} \partial_{\rho_k} (\rho_k^2 \partial_{\rho_k} s_k) & \partial_{\rho_k, e_k} s_k \\ \partial_{\rho_k, e_k} s_k & \partial_{e_k, e_k} s_k \end{bmatrix}. \end{aligned}$$

Eq. (21) is used to prove the entropy minimum principle: assuming that  $s_k$  reaches its minimum value in  $r_{min}(t)$  at each time t, the gradient,  $\nabla s_k$ , and Laplacian,  $\Delta s_k$ , of the entropy are null and positive at this particular point, respectively. Furthermore, it is recalled that the viscosity coefficients  $\mu_k$  and  $\kappa_k$  are positive by definition. Then, because the terms in the right-hand-side of Eq. (21) are proven either positive or null when the entropy reaches a minimum value, the entropy minimum principle holds for each phase k, independently of the definition of the dissipative term  $l_k$ , such as:

$$\alpha_k \rho_k A \partial_t s_k(\mathbf{r}_{min}, t) \ge 0 \Rightarrow \partial_t s_k(\mathbf{r}_{min}, t) \ge 0$$

#### Do we need to make the above statement a theorem or property?

It remains to obtain a definition for the dissipative term  $l_k$  used in the volume fraction equation Eq. (10a). A way to achieve this is to consider the volume fraction equation, by itself and notice that it is an hyperbolic equation with eigenvalue  $u_{int}$ . An entropy equation can be derived and used to prove the entropy minimum principle by properly choosing the dissipative term [16]. The objective is to ensure positivity of the volume fraction and also uniqueness of the weak solution. Following the work of Guermond et al. in [17, 18], it can be shown that a dissipative term ensuring positivity and uniqueness of the weak solution for the volume fraction equation, is of the form  $l_k = \beta_k A \nabla \alpha_k$ , where

 $\beta_k$  is a positive viscosity coefficient. The dissipative term is proportional to the area A for consistency with the other terms of the volume fraction equation Eq. (10a).

All of the dissipative terms are now defined and recalled here:

$$\boldsymbol{l}_k = \beta_k A \boldsymbol{\nabla} \alpha_k \tag{22a}$$

$$\boldsymbol{f}_k = \alpha_k A \kappa_k \boldsymbol{\nabla} \rho_k + \rho_k A \boldsymbol{l}_k \tag{22b}$$

$$\boldsymbol{g}_k = \alpha_k A \mu_k \rho \boldsymbol{\nabla}^s \boldsymbol{u}_k \tag{22c}$$

$$\boldsymbol{h}_{k} = \alpha_{k} A \kappa_{k} \nabla (\rho e)_{k} + \boldsymbol{u}_{k} : \boldsymbol{g}_{k} - \frac{||\boldsymbol{u}_{k}||^{2}}{2} \boldsymbol{f}_{k} + (\rho e)_{k} \boldsymbol{l}_{k}$$
(22d)

At this point, some remarks are in order:

- 1. The viscous regularization given in Eq. (22) for the multi-D seven-equation model, is equivalent to the parabolic regularization [19] when assuming  $\beta_k = \kappa_k = \mu_k$  and  $\mathbb{F}(\boldsymbol{u}_k) = \alpha_k \rho_k \kappa_k \nabla \boldsymbol{u}_k$ . However, decoupling between the regularization on the velocity and on the density in the momentum equation is important to make the regularization rotation invariant but also to ensure well-scaled dissipative terms for a wide range of Mach number as was shown in [15] for the multi-D Euler equations.
- 2. The dissipative term  $l_k$  requires the definition of a new viscosity coefficient  $\beta_k$ . It was shown that this viscosity coefficient is independent of the other viscosity coefficients  $\mu_k$  and  $\kappa_k$ . Its definition should account for the eigenvalue associated with the void fraction equation  $u_{int}$ .
- 3. The dissipative term  $f_k$  is a function of  $l_k$ . Thus, all of the other dissipative terms are also functions of  $l_k$ .
- 4. The partial derivatives  $(s_e)_k$  and  $(s_{\rho_k})_k$  can be computed using the definition provided in Eq. (16) and are functions of the thermodynamic variables: pressure, temperature and density.
- 5. All of the dissipative terms are chosen to be proportional to the void fraction  $\alpha_k$  and the cross-sectional area A, but the one in the volume fraction equation that is only proportional to A. For instance,  $\alpha_k A \nabla \rho_k$  is the flux of the dissipative term in the continuity equation through the phasic area,  $\alpha_k A$ , seen by the phase k. When one of the phases disappears, the dissipative terms must go to zero for consistency. On the other hand, when  $\alpha_k$  goes to one, the single-phase Euler equations with proper viscous regularization must be recovered.
- 6. Compatibility of the viscous regularization proposed in Eq. (22) with the generalized entropies identified in Harten et al. [20] has not been investigated yet. However, it is believed that the entropy inequalities still holds because of the similarities of the entropy residual for the multi-D seven-equation model with the entropy residual derived in the single phase flow case [13].

At this point in the paper, we have derived a viscous regularization for the multi-D seven-equation two-phase flow model that ensures positivity of the entropy residual, uniqueness of the numerical solution when assuming concavity of the 169 phasic entropy  $s_k$ , and is consistent with the viscous regularization derived 170 for the multi-D Euler equations [13, 15] in the limit  $\alpha_k \to 1$ . The viscous 171 regularization involves a set of three viscosity coefficients for each phase,  $\mu_k$ , 172  $\kappa_k$  and  $\beta_k$ , that are assumed positive. Definition of the viscosity coefficients is 173 now required to complete the numerical stabilization method. Since the focus of this paper is the entropy viscosity method, the viscosity coefficients will be 175 defined function of the entropy residual in Section 4. However, one can also devise a definition for the viscosity coefficients  $\mu_k$  and  $\kappa_k$  by analogy to Lapidus 177 [21, 22] or some pressure-based methods [23] used for the single-phase Euler 178 equations. On the other hand, the viscosity coefficient,  $\beta_k$ , for the volume 179 fraction equation should rely on artificial dissipation stabilization methods used for scalar hyperbolic equations. 181

**Remark.** Through the derivations of the viscous regularization, it was noted that another set of dissipative terms  $f_k$  and  $l_k$  would also ensures positivity of the entropy residual:

$$\boldsymbol{l}_{k} = \beta_{k} T_{k} \left[ \frac{\rho_{k}}{P_{k} + \rho_{k} e_{k}} \boldsymbol{\nabla} \left( \frac{P_{k}}{\rho_{k} e_{k}} \right) - \frac{1}{P_{k}} \boldsymbol{\nabla} \rho_{k} \right]$$
 (23a)

$$\boldsymbol{f}_{k} = \kappa_{k} \boldsymbol{\nabla} \rho_{k} + \frac{\rho_{k}^{2}(s_{\rho})_{k}}{(\rho s_{\rho} - e s_{e})_{k}} \boldsymbol{l}_{k}$$
 (23b)

However, the definition of  $l_k$  proposed in Eq. (23a) was not considered as valid for the following reasons: positivity of the volume fraction cannot be achieved and the parabolic regularization is not retrieved when assuming equal viscosity coefficients.

#### 4. A definition of the viscosity coefficients for all Mach flows

- non-dimensionalize the equations but use  $P_{\infty}$  for the pressure instead of  $(\rho c^2)_{\infty}$
- introduce a new Pechlet number for  $\beta$ : its behavior should be the same as the Pechlet number for  $\kappa$
- two cases: zero and infinite relaxation coefficients
- derive the normalization parameters for the isentropic and non-isentropic flows
- discussion about the

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When working with artificial dissipative numerical stabilization methods, great care needs to be carried to the definition of the viscosity coefficients that will determine the accuracy of the method. Generally speaking, sufficient artificial viscosity should be added into the shock and discontinuity regions to prevent spurious oscillations from forming, while little dissipation is added when the numerical solution is smooth. Such requirements can be achieved by tracking shocks and discontinuities in the numerical solutions. When dealing with fluid equations, the low-mach asymptotic limit also has to be accounted for in the definition of the viscosity coefficients in order to ensure well-scaled dissipative terms [24, 25, 26]. Also, because each phase can experience different flow regime (the gas phase is supersonic whereas the liquid phase remains subsonic), it is chosen to work with three distinct viscosity coefficients for each phase. The purpose of this section is to derive a definition for the phasic viscosity coefficients,  $\mu_k$ ,  $\kappa_k$  and  $\beta_k$ , that ensures the correct numerical solution in the low-mach limit, can accurately resolves shocks in transonic and supersonic flows and is also consistent with the definition of the viscosity coefficients devised for the single-phase Euler equations in the limit  $\alpha_k \to 1$ . As a result, the approach used in [15] will be applied here in this section.

#### 4.1. Definition of the viscosity coefficients

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In the entropy viscosity method, each viscosity coefficient is function of an upper and a lower bound that are referred to as first-order viscosity coefficient and entropy viscosity coefficient (high-order coefficient), respectively, as shown in Eq. (24). The first-order viscosity coefficient is denoted by the subscript max and is defined proportional to the largest local eigenvalue so that the stabilization scheme becomes over-dissipative and smooth out all discontinuities. The entropy viscosity coefficient is set proportional to an entropy residual and jumps of quantities to determine, and denoted by the subscript e.

$$\beta_{k}(\mathbf{r},t) = \min \left( \beta_{e,k}(\mathbf{r},t), \beta_{max,k}(\mathbf{r},t) \right),$$

$$\mu_{k}(\mathbf{r},t) = \min \left( \mu_{e,k}(\mathbf{r},t), \mu_{max,k}(\mathbf{r},t) \right),$$

$$\kappa_{k}(\mathbf{r},t) = \min \left( \kappa_{e,k}(\mathbf{r},t), \kappa_{max,k}(\mathbf{r},t) \right),$$
(24)

where all of the variables are locally defined. We now define the first-order viscosity coefficients and will focus first on the phasic viscosity coefficients  $\kappa_k$  and  $\mu_k$  that are untimely linked to the mass, momentum and energy equations. These two viscosity coefficients are involved in dissipative terms that identical to the ones obtained for the single-phase Euler equations [13, 15] when seeing the term  $\alpha_k A$  as a pseudo cross-section. Thus, it is chosen to define the corresponding first-order viscosity coefficients proportional to the local largest eigenvalue  $||u_k|| + c_k$  as follows:

$$\kappa_{max,k}(\boldsymbol{r},t) = \mu_{max,k}(\boldsymbol{r},t) = \frac{h}{2} \left( ||\boldsymbol{u}_k||(\boldsymbol{r},t) + c_k(\boldsymbol{r},t) \right), \tag{25}$$

where h is the grid size. It remains to define the first-order viscosity coefficient,  $\beta_{max}$ , used in the volume fraction equation. Because the volume fraction equation can be treated as a hyperbolic scalar equation with an unique eigenvalue  $u_{int}$ , the first-order viscosity coefficient is defined by analogy with Burger's equation [17, 18] as follows:

$$\beta_{max,k}(\mathbf{r},t) = \frac{h}{2}||\mathbf{u}_{int}(\mathbf{r},t)||. \tag{26}$$

After defining the first-order viscosity coefficients for each phase, we focus our attention to the entropy viscosity coefficients denoted by the subscript e in Eq. (24). We first choose to investigate the definitions of  $\mu_{e,k}$  and  $\kappa_{e,k}$ . The entropy viscosity coefficients are set proportional to the entropy residual given in Eq. (27), that is known to be positive and peaked in the shock region.

$$R_k(\mathbf{r},t) := \frac{\mathrm{D}s_k}{\mathrm{D}t} = \partial_t s_k + \mathbf{u}_k \cdot \nabla s_k \tag{27}$$

It is also accounted for the jumps of quantities that will be determined further. The objective is to be able to track spatially and temporally any shock and discontinuity forming in the computational domain. In [15], it was demonstrated the usefulness of recasting the entropy residual as a function of pressure, velocity, density and speed of sound as shown in Eq. (28). The alternative expression of the entropy residual denoted by  $\widetilde{R}_k(\mathbf{r},t)$ , no longer requires an analytical expression of the entropy  $s_k$  and experiences the same variations (in absolute value) as the original definition of the entropy residual (Eq. (27)).

$$R_{k}(\mathbf{r},t) = \frac{\mathrm{D}s_{k}}{\mathrm{D}t} = \frac{(s_{e})_{k}}{(P_{e})_{k}} \left(\underbrace{\frac{\mathrm{D}P_{k}}{\mathrm{D}t} - c_{k}^{2} \frac{\mathrm{D}\rho_{k}}{\mathrm{D}t}}_{\widetilde{R}_{k}(\mathbf{r},t)}\right), \tag{28}$$

Using the new expression of the entropy residual  $\widetilde{R}_k$ , we now propose a definition, given in Eq. (29), for the phasic entropy viscosity coefficients  $\mu_{e,k}$  and  $\kappa_{e,k}$  that also accounts for jumps,  $J_k$ , of some function of the pressure and density for generality purpose. The jump helps at tracking contact waves or discontinuities other than shock that are not seen by the entropy residual. Its definition will be detailed in SECTION. A distinct normalization parameter is also introduced for each viscosity coefficient that is used for dimensionality purpose: a quick dimensional study of the dissipative terms shows that the viscosity coefficients are kinematic viscosity  $(m^2 \cdot s^{-1})$ . Thus, the normalization parameters has units in pressure and its final definition will be determined by a low-Mach asymptotic limit of Eq. (10) in order to ensure well-scaled dissipative terms.

$$\mu_{e,k}(\boldsymbol{r},t) = h^2 \frac{\max\left(\left|\widetilde{R}_k(\boldsymbol{r}_q,t)\right|,\left|\left|J_k^{\mu}\right|\right|\right)}{\operatorname{norm}_{P,k}^{\mu}},$$
(29a)

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$$\kappa_{e,k}(\boldsymbol{r},t) = h^2 \frac{\max\left(|\widetilde{R}_k(\boldsymbol{r}_q,t)|,||J_k^{\kappa}||\right)}{\operatorname{norm}_{P,k}^{\kappa}}.$$
 (29b)

It remains to define the entropy viscosity coefficient  $\beta_e$ . For the purpose of this paragraph, let us consider the scalar volume fraction equation and assume that the interface velocity  $u_{int}$  is given. Because it is a scalar hyperbolic equation, it is proposed to define the entropy viscosity coefficients on the same model as what is done for Burger's equation [17, 18]. Thus, the entropy viscosity viscosity coefficient  $\beta_e$  is defined as a function of an entropy residual,  $R_k^{\alpha}$ , derived from the volume fraction equation for phase k, and the jump of a function of the volume fraction,  $J_k^{\alpha}$ , as shown in Eq. (30).

$$\beta_{e,k}(\boldsymbol{r},t) = h^2 \frac{\max\left(\left|R_k^{\alpha}(\boldsymbol{r}_q,t)\right|,\left|\left|J_k^{\alpha}\right|\right|\right)}{\operatorname{norm}_{\alpha,k}^{\beta}}$$
(30)

We also introduced a normalization parameter,  $\operatorname{norm}_{\alpha,k}^{\beta}$ , whom definition will be further investigated. To derive the entropy residual,  $R_{\alpha,k}$ , we consider the volume fraction equation for phase k with its viscous regularization and assume the existence of an entropy denoted by  $\eta_k(\alpha_k)$  [16]:

$$\partial_t (A\alpha_k) + A \boldsymbol{u}_{int} \cdot \boldsymbol{\nabla} \alpha_k = \boldsymbol{\nabla} \cdot (\beta_k A \boldsymbol{\nabla} \alpha_k)$$
 (31)

After multiplying by  $\frac{d\eta(\alpha_k)}{d\alpha_k}$  and using the chain rule, an expression for the entropy equation is obtained:

$$\underbrace{\partial_t \left( A \eta(\alpha_k) \right) + A \boldsymbol{u}_{int} \cdot \boldsymbol{\nabla} \eta(\alpha_k)}_{R^{\alpha}} = \frac{\mathrm{d}\eta(\alpha_k)}{\mathrm{d}\alpha_k} \boldsymbol{\nabla} \cdot (\beta_k A \boldsymbol{\nabla} \alpha_k) \tag{32}$$

The entropy residual,  $R_k^{\alpha}$ , is defined as the left hand side of Eq. (32) and is known to be peaked in the shock region and positive when assuming convexity of the entropy  $\eta_k$  with respect to  $\alpha_k$  [16]. Such a behavior is identical to the entropy residual  $\tilde{R}_k$  defined in Eq. (28), and will allow detection of the shock wave when used in the definition of the entropy viscosity coefficient  $\beta_{e,k}$ . At this point of the paper, the definition of the viscosity coefficients are not finalized: the jumps and normalization parameters still have to be defined. Details regarding the definition of the jump will be given in Section 5. The normalization parameters are derived from a low-Mach asymptotic limit analysis which is the purpose of the next section.

#### 4.2. Low-Mach asymptotic limit of the seven-equation model

Developing a numerical method for fluid equations require to investigate the low-Mach asymptotic limit. In this particular limit, numerical methods developed for transonic and supersonic flows usually fail due to ill-scaled dissipative terms. A fix is found by performing a low-Mach asymptotic limit to ensure well-scaled dissipative terms [24, 25, 26]. Then, it is proposed to perform a low-Mach asymptotic limit to derive an expression for the phasic normalization parameters introduced in Section 4.1. Two limit 1-D cases are considered: the relaxation coefficients are set to (i) zero and (ii) to very large values. In the former case, the two phases do not interact and each phase simply flows through

a given geometry of pseudo cross-section  $\alpha_k A$ . In the later case, the infinite relaxation coefficients make the seven-equation two-phase model degenerates into the five-equation model of Kapila by ensuring pressure and velocity equilibrium. For each case (i) and (ii), two limit cases (a) and (b) will be considered to determine appropriate scaling for the entropy viscosity coefficients so that the dissipative terms remain well-scaled for two limit cases: (a) the isentropic low-Mach limit where the seven-equation model degenerate to an incompressible system of equations in the low-Mach limit and (b) the non-isentropic limit with formation of shocks. In the low-Mach limit, the isentropic limit of the sevenequation model with viscous regularization should yield incompressible fluid flow solutions, namely, that the phasic pressure fluctuations are of the order  $M_k^2$  and that the velocity satisfies the divergence constraint  $\nabla \cdot (\vec{u}_0)_k = 0$  [24, 25, 26]. For non-isentropic situations, shocks may form for any value of Mach number and the minimum entropy principle should still be satisfied so that numerical oscillations, if any, be controlled by the entropy viscosity method independently of the value of the Mach number. A total of four different cases will be studied and for each case the scaling of the numerical adimensional numbers will be given along with the definition of the normalization parameters defined in Section 4.1 for each viscosity coefficients.

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The first step in the study of the limit cases (i) and (ii) is to re-write each system of equations in a non-dimensional manner. To do so, the following variables are introduced for each phase k:

$$\rho_{k}^{*} = \frac{\rho_{k}}{\rho_{k,\infty}}, \ u_{k}^{*} = \frac{u_{k}}{u_{k,\infty}}, \ P_{k}^{*} = \frac{P_{k}}{\rho_{k,\infty}c_{k,\infty}^{2}}, \ E_{k}^{*} = \frac{E_{k}}{c_{k,\infty}^{2}}, \ x^{*} = \frac{x}{L_{\infty}},$$

$$t_{k}^{*} = \frac{t_{k}}{L_{\infty}/u_{k,\infty}}, \ \mu_{k}^{*} = \frac{\mu_{k}}{\mu_{k,\infty}}, \ \kappa_{k}^{*} = \frac{\kappa_{k}}{\kappa_{k,\infty}}, \ P_{int}^{*} = \frac{P_{int}}{P_{int,\infty}},$$

$$u_{int}^{*} = \frac{u_{int}}{u_{int,\infty}}, \ \bar{P}_{int}^{*} = \frac{\bar{P}_{int}}{\bar{P}_{int,\infty}}, \ \bar{u}_{int}^{*} = \frac{\bar{u}_{int}}{\bar{u}_{int,\infty}},$$

$$(33)$$

where the subscript  $\infty$  denote the far-field or stagnation quantities and the superscript \* stands for the non-dimensional variables. The far-field reference quantities are chosen such that the dimensionless flow quantities are of order 1. The stagnation quantities for the pressure and velocity interfacial variables will be specified for each case. The reference Mach number is given by

$$M_{k,\infty} = \frac{u_{k,\infty}}{c_{k,\infty}}. (34)$$

We start the low-Mach analysis with case (i) and give the system of equations with viscous regularization that is used when assuming zero relaxation coefficients:

$$\partial_t \left( \alpha_k \rho_k A \right) + \nabla \cdot \left( \alpha_k \rho_k \mathbf{u}_k A \right) = \nabla \cdot \left( \kappa_k \nabla \rho_k \right) \tag{35a}$$

$$\partial_{t} \left( \alpha_{k} \rho_{k} \boldsymbol{u}_{k} A \right) + \boldsymbol{\nabla} \cdot \left[ \alpha_{k} A \left( \rho_{k} \boldsymbol{u}_{k} \otimes \boldsymbol{u}_{k} + P_{k} \mathbb{I} \right) \right] = \alpha_{k} P_{k} \boldsymbol{\nabla} A + P_{int} A \boldsymbol{\nabla} \alpha_{k} + \boldsymbol{\nabla} \cdot \left[ \mu_{k} \rho_{k} \boldsymbol{\nabla}^{s} \vec{u} + \kappa_{k} \vec{u}_{k} \otimes \boldsymbol{\nabla} \rho_{k} \right]$$
(35b)

$$\partial_t \left( \alpha_k \rho_k E_k A \right) + \nabla \cdot \left[ \alpha_k A \boldsymbol{u}_k \left( \rho_k E_k + P_k \right) \right] = P_{int} A \boldsymbol{u}_{int} \cdot \nabla \alpha_k - + \nabla \cdot (\boldsymbol{h}_k + \boldsymbol{u} \cdot \boldsymbol{g}_k)$$
(35c)

$$\partial_t \left( \alpha_k A \right) + \boldsymbol{u}_{int} A \boldsymbol{\nabla} \alpha_k = \boldsymbol{\nabla} \cdot \boldsymbol{l}_k \tag{35d}$$

Then, the scaled equations for the phase k with viscous regularization are:

$$\partial_t (\alpha_k \rho_k A) + \nabla \cdot (\alpha_k \rho_k \boldsymbol{u}_k A) = \frac{1}{\text{P\'e}_{k,\infty}} \nabla \cdot (\kappa_k \nabla \rho_k)$$
 (36a)

$$\partial_{t} \left( \alpha_{k} \rho_{k} \boldsymbol{u}_{k} A \right) + \boldsymbol{\nabla} \cdot \left[ \alpha_{k} A \left( \rho_{k} \boldsymbol{u}_{k} \otimes \boldsymbol{u}_{k} + P_{k} \mathbb{I} \right) \right] = \alpha_{k} P_{k} \boldsymbol{\nabla} A + P_{int} A \boldsymbol{\nabla} \alpha_{k} + \boldsymbol{\nabla} \cdot \boldsymbol{g}_{k}$$
(36b)

$$\partial_t \left( \alpha_k \rho_k E_k A \right) + \nabla \cdot \left[ \alpha_k A \boldsymbol{u}_k \left( \rho_k E_k + P_k \right) \right] = P_{int} A \boldsymbol{u}_{int} \cdot \nabla \alpha_k - + \nabla \cdot (\boldsymbol{h}_k + \boldsymbol{u} \cdot \boldsymbol{g}_k)$$
(36c)

$$\partial_t \left( \alpha_k A \right) + \boldsymbol{u}_{int} A \boldsymbol{\nabla} \alpha_k = \boldsymbol{\nabla} \cdot \boldsymbol{l}_k \tag{36d}$$

#### 5. Discretizations and Solution Techniques

In this section, we briefly describe the spatial and temporal discretizations and the solution techniques used to solve the system of equations Eq. (10). For conciseness, we re-write the system of equations in the following form:

$$\partial_t \mathbf{U}_k + \nabla \cdot \mathbf{F}_k \left( \mathbf{U}_k \right) = \mathbf{R}_k \left( \mathbf{U}_k \right) + \mathbf{N}_k \left( \mathbf{U}_k \right) + \nabla \cdot \mathbf{D}_k \left( \mathbf{U}_k \right) \nabla \mathbf{U}_k \tag{37}$$

where  $\mathbf{U}_k = [(\alpha A)_k, (\alpha \rho A)_k, (\alpha \rho \mathbf{u} A)_k, (\alpha \rho E A)_k]^T$  is the solution vector,  $\mathbf{F}_k(\mathbf{U}_k)$ denotes the inviscid flux,  $\nabla \cdot D_k(\mathbf{U}_k) \nabla \mathbf{U}_k$  is the dissipative flux and  $\mathbf{N}_k(\mathbf{U}_k)$ and  $\mathbf{R}_k(\mathbf{U}_k)$  contain the non-conservative and relaxation terms, respectively.

$$\mathbf{F} \equiv \begin{bmatrix} 0 \\ (\alpha \rho u A)_k \\ [\alpha (\rho u^2 + P) A]_k \\ [\alpha u(\rho E + P) A]_k \end{bmatrix}, \mathbf{N} \equiv \begin{bmatrix} -A \mathbf{u}_{int} \cdot \nabla \alpha_k \\ 0 \\ \alpha_k P_k \nabla A + P_{int} A \nabla \alpha_k \\ P_{int} A \mathbf{u}_{int} \cdot \nabla \alpha_k \end{bmatrix}$$

and 
$$\mathbf{R} \equiv \begin{bmatrix} A\mu_P \left(P_k - P_j\right) & & & \\ 0 & & & \\ A\lambda_u \left(\boldsymbol{u}_j - \boldsymbol{u}_k\right) & & \\ -\bar{P}_{int}A\mu_P \left(P_k - P_j\right) + \bar{u}_{int}A\lambda_u \left(\boldsymbol{u}_j - \boldsymbol{u}_k\right) \end{bmatrix}.$$

310 5.1. Spatial and Temporal Discretizations

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The system of equations given in Eq. (37) is discretized using a continuous Galerkin finite element method and temporal integrators available through the MOOSE multiphysics framework [27].

#### 5.1.1. Continuous Finite Elements

In order to apply the continuous finite element method, Eq. (37) is multiplied by a test function  $\mathbf{W}(r)$ , integrated by parts and each integral is decomposed into a sum of integrals over each element K of the discrete mesh  $\Omega$ . The following weak form is obtained:

$$\sum_{K} \int_{K} \partial_{t} \mathbf{U} \mathbf{W} - \sum_{K} \int_{K} \mathbf{F}(\mathbf{U}) \cdot \nabla \mathbf{W} + \int_{\partial \Omega} \mathbf{F}(\mathbf{U}) \cdot n \mathbf{W} - \sum_{K} \int_{K} (\mathbf{N}(\mathbf{U}) + \mathbf{R}(\mathbf{U})) \mathbf{W}$$
$$+ \sum_{K} \int_{K} D(\mathbf{U}) \nabla \mathbf{U} \cdot \nabla \mathbf{W} - \int_{\partial \Omega} D(\mathbf{U}) \nabla \mathbf{U} \cdot n \mathbf{W} = 0. \quad (38)$$

The integrals over the elements K are evaluated using a numerical quadrature. The MOOSE framework provides a wide range of test functions and quadrature rules. Linear Lagrange polynomials are employed as test functions in the results section. Second-order spatial convergence will be demonstrated for smooth solutions.

#### 5.1.2. Temporal integration

The MOOSE framework offers both first- and second-order explicit and implicit temporal integrators. In all of the numerical examples presented in Section 6, the temporal derivative will be evaluated using the second-order, backward difference temporal integrator BDF2. By considering three consecutive solutions,  $\mathbf{U}^{n-1}$ ,  $\mathbf{U}^n$  and  $\mathbf{U}^{n+1}$ , at times  $t^{n-1}$ ,  $t^n$  and  $t^{n+1}$ , respectively, BDF2 can be expressed as:

$$\int_{K} \partial_{t} \mathbf{U} \mathbf{W} = \int_{K} \left( \omega_{0} \mathbf{U}^{n+1} + \omega_{1} \mathbf{U}^{n} + \omega_{2} \mathbf{U}^{n-1} \right) \mathbf{W},$$
 (39)

with

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$$\omega_0 = \frac{2\Delta t^{n+1} + \Delta t^n}{\Delta t^{n+1} \left(\Delta t^{n+1} + \Delta t^n\right)}, \ \omega_1 = -\frac{\Delta t^{n+1} + \Delta t^n}{\Delta t^{n+1} \Delta t^n},$$
 and 
$$\omega_2 = \frac{\Delta t^{n+1}}{\Delta t^n \left(\Delta t^{n+1} + \Delta t^n\right)}$$

where  $\Delta t^n = t^n - t^{n-1}$  and  $\Delta t^{n+1} = t^{n+1} - t^n$ .

#### 5.2. Boundary conditions

Boundary conditions for the seven-equation model are challenging because of the wave-dominated nature of the equations but also because of the non-conservative form of the volume fraction equation. Unlike the continuity, momentum and energy equations of each phase, the flux of the volume fraction equation is not integrated by part because not under conservative form, and thus, does not stem a boundary flux. Then, the boundary condition for the volume fraction equation (Eq. (1d)) is treated independently of the other equations (continuity, momentum and energy for each phase) for two reasons: (i) it is a

simple advection equation with the real eigenvalue  $u_{int}$ , and (ii), the hyperbolic flux,  $u_{int} \cdot \nabla \alpha_k$ , is not integrated by part since not under a conservative form. The sign of the dot product between the eigenvalue and the outward normal to the boundary,  $u_{int} \cdot n$ , determines the nature of the boundary: negative for an inlet and positive for an outlet. For the later case, the physical information exits the computational domain and does not require any particular treatment. In the former case, the physical information enters the computational domain which requires to specify a value for the volume fraction. Since there is no flux at the boundary coming from the integration by part of the hyperbolic flux, the boundary value is imposed by using a Dirichlet boundary condition in the volume fraction equation. Our implementation of the boundary conditions for the continuity, momentum and energy equations, is inspired by the method described in [3] and was adapted for a time implicit solver [14]. The boundary type is identified from the study of the sign of the eigenvalues that depends on the Mach number. The numerical results presented in Section 6 were all obtained by using subsonic stagnation and static pressure boundary conditions for the inlet and outlet, respectively. The boundary flux is computed from the supplied variables at the boundary and also by iterating on a given number of variables (depending on the sign of the eigenvalues) though the implicit solver to transmit information from inside the computational domain toward the boundary.

The artificial diffusion coefficient  $D(\mathbf{U})$  is set to zero at the boundary of the computational domain so that the boundary term  $\int_{\partial\Omega} D(\mathbf{U}) \nabla \mathbf{U} \cdot \mathbf{n} \mathbf{W}$  stemming from the integration by parts of the artificial dissipative terms in Eq. (38) is ignored.

#### 5.3. Solver

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A Jacobian-free-Newton-Krylov (JFNK) method is used to solve for the solution at the end of each time step. An approximate Jacobian matrix of the discretized equations was derived and implemented. Obtaining the matrix entries requires that the partial derivatives of pressure with respect to the conservative variables be known (this is relatively simple for the stiffened and ideal gas equations of state but may be more complex for general equations of state). The contributions of the artificial dissipative terms to the Jacobian matrix are approximated by lagging the viscosity coefficients (computing them with the previous solution). For instance, this is shown in Eq. (40) for the dissipative terms present in the continuity equation:

$$\frac{\partial}{\partial \mathbf{U}} \left( \kappa \nabla \rho \cdot \nabla W \right) \simeq \kappa \nabla \cdot \frac{\partial \rho}{\partial \mathbf{U}} \nabla W, \tag{40}$$

where **U** denotes any of the conservative variables and W denotes the component of **W** associated with the continuity equation. In the above, we have neglected  $\frac{\partial \kappa}{\partial \mathbf{U}}$ .

#### 6. 1-D numerical results

• simple advection problem

- shock tube with two independent fluids: exact solution and could do convergence test for this particular test
- shock tube with infinite relaxation coefficients
  - 1-D nozzle with two independent fluids
- 1-D nozzle with infinite relaxation coefficients
  - 1-D nozzle with infinite relaxation coefficients, mass and heat transfer

#### 383 References

- [1] A. K. Kapila, R. Menikoff, J. B. B. S. F. Son, D. S. Stewart, Two-phase
   modeling of deflagration-to-detonation transition in granular materials,
   Phys. Fluids (2001) 3002–3024.
- <sup>387</sup> [2] I. Toumi, An upwind numerical method for two-fluids two-phases flow models, Nucl. Sci. Eng. (1996) 147–168.
- [3] R. Berry, R. Saurel, O. LeMetayer, The discrete equation method (dem)
   for fully compressible, two-phase flows in ducts of spatially varying cross section, Nuclear Engineering and Design 240 (2010) 3797–3818.
- R. Abgrall, How to prevent pressure oscillations in multicomponent flow calcuations: a quasi conservative appraoch, J. Comput. Phys (2002) 125–150.
- <sup>395</sup> [5] R. Saurel, R. Abgrall, A multiphase godunov method for compressible multifluid and multiphase flows, J. Comput Physics (2001) 425–267.
- <sup>397</sup> [6] R. Saurel, O. Lemetayer, A multiphase model for compressible flows with interfaces, shocks, detonation waves and cavitation, J. Comput Physics (2001) 239–271.
- [7] Q. Li, H. Feng, T. Cai, C. Hu, Difference scheme for two-phase flow, Appl
   Math Mech (2004) 536.
- [8] A. Zein, M. Hantke, G. Warnecke, Modeling phase transition for compress ible two-phase flows applied to metastabe liquids, J. Comput Physics (2010)
   2964.
- [9] A. Ambroso, C. Chalons, P.-A. Reviart, A godunov-type method for the seven-equation model of compressible multiphase mixtures, Comput. Fluids (2012) 67–91.
- [10] R. A. Berry, M. Delchini, J. Ragusa, Relap-7 numrerical stabilization: Entropy viscosity method, Tech. Rep. INL/EXT-14-32352, Idaho National Laboratory, USA (2014).

- [11] R. Saurel, F. Petitpas, R. A. Berry, Simple and efficient relaxation methods
   for interfaces separating compressible fluids, cavitating flows and shocks in
   multiphase mixtures, J. of Computational Physics 228 (2009) 1678–1712.
- [12] J. M. Herrard, O. Hurisse, A simple method to compute standard two-fluid
   models, Int. J. of Computational Fluid Dynamics 19 (2005) 475–482.
- [13] J. L. Guermond, B. Popov, Viscous regularization of the euler equations
   and entropy principles, under review.
- 418 [14] M. Delchini, Extension of the entropy viscosity method to multi-d euler equations and the seven-equation two-phase model, Tech. rep., Texas A& M University, USA (2014).
- [15] M. Delchini, J. Ragusa, R. Berry, Entropy-based viscosity regularization for the multi-dimensional euler equations in low-mach and transonic flows, under review.
- [16] R. Leveque, Numerical Methods for Conservation Laws, Birkhuser Basel, Zurich, Switzerland, 1990.
- [17] J. L. Guermond, R. Pasquetti, Entropy viscosity method for nonlinear conservation laws, Journal of Comput. Phys 230 (2011) 4248–4267.
- <sup>428</sup> [18] J. L. Guermond, R. Pasquetti, Entropy viscosity method for high-order approximations of conservation laws, Lecture Notes in Computational Science and Engineering 76 (2011) 411–418.
- [19] B. Perthane, C. W. Shu, On positivity preserving finite volume schemes for euler equations, Numer. Math. 73 (1996) 119–130.
- [20] A. Harten, L. P. Franca, M. Mallet, Convex entropies and hyperbolicity for general euler equations, SIAM J Numer Anal 6 (1998) 2117–2127.
- [21] A. Lapidus, A detached shock calculation by second order finite differences,
   J. Comput. Phys. 2 (1967) 154–177.
- [22] J. Donea, A. Huerta, Finite Element Methods for Flow Problems, Oxford
   University Press, 2003.
- [23] R. Lohner, Applied CFD Techniques: an Introduction based on Finite Element Methods, 2<sup>nd</sup> Edition Wiley, 2003.
- <sup>441</sup> [24] H. Guillard, C. Viozat, On the behavior of upwind schemes in the low mach number limit, Computers & Fluids 28 (1999) 63–86.
- [25] E. Turkel, Preconditioned techniques in computational fluid dynamics, Annu. Rev. Fluid Mech. 31 (1999) 385–416.
- [26] J. S. W. D. L, Darmofal, J. Peraire, The solution of the compressible euler equations at low mach numbers using a stabilized finite element algorithm,
   Comput. Methods Appl. Mech. Engrg. 190 (2001) 5719–5737.

[27] D. Gaston, C. Newsman, G. Hansen, D. Lebrun-Grandie, A parallel computational framework for coupled systems of nonlinear equations, Nucl. Eng. Design 239 (2009) 1768–1778.

## Appendix A Entropy equation for the multi-D seven equation model without viscous regularization

This appendix provides the steps that lead to the derivation of the phasic entropy equation of the seven-equation model [3]. For the purpose of this dissertation, two phases are considered and denoted by the indexes j and k. In the seven-equation model, each phase obeys to the following set of equations (Eq. (41)):

$$\partial_t \left( \alpha_k A \right) + A \boldsymbol{u}_{int} \cdot \boldsymbol{\nabla} \alpha_k = A \mu \left( P_k - P_i \right) \tag{41a}$$

$$\partial_t \left( \alpha_k \rho_k A \right) + \nabla \cdot \left( \alpha_k \rho_k \boldsymbol{u}_k A \right) = 0 \tag{41b}$$

$$\partial_{t} (\alpha_{k} \rho_{k} \boldsymbol{u}_{k} A) + \nabla \cdot [\alpha_{k} A (\rho_{k} \boldsymbol{u}_{k} \otimes \boldsymbol{u}_{k} + P_{k} \mathbb{I})] = \alpha_{k} P_{k} \nabla A + P_{int} A \nabla \alpha_{k} + A \lambda (\boldsymbol{u}_{j} - \boldsymbol{u}_{k})$$
(41c)

$$\partial_{t} \left( \alpha_{k} \rho_{k} E_{k} A \right) + \nabla \cdot \left[ \alpha_{k} A \boldsymbol{u}_{k} \left( \rho_{k} E_{k} + P_{k} \right) \right] = P_{int} A \boldsymbol{u}_{int} \cdot \nabla \alpha_{k} - \mu \bar{P}_{int} \left( P_{k} - P_{j} \right) + \bar{\boldsymbol{u}}_{int} A \lambda \left( \boldsymbol{u}_{j} - \boldsymbol{u}_{k} \right)$$
(41d)

where  $\rho_k$ ,  $u_k$ ,  $E_k$  and  $P_k$  are the density, the velocity, the specific total energy and the pressure of  $k^{th}$  phase, respectively. The pressure and velocity relaxation parameters are denoted by  $\mu_P$  and  $\lambda_u$ , respectively. The variables with index int correspond to the interfacial variables and a definition is given in Eq. (42). The cross section A is only function of space:  $\partial_t A = 0$ .

$$\begin{cases}
P_{int} = \bar{P}_{int} - \frac{\nabla \alpha_k}{||\nabla \alpha_k||} \frac{Z_k Z_j}{Z_k + Z_j} \left( \boldsymbol{u}_k - \boldsymbol{u}_j \right) \\
\bar{P}_{int} = \frac{Z_k P_j + Z_j P_k}{Z_k + Z_j} \\
\boldsymbol{u}_{int} = \bar{\boldsymbol{u}}_{int} - \frac{\nabla \alpha_k}{||\nabla \alpha_k||} \frac{P_k - P_j}{Z_k + Z_j} \\
\bar{\boldsymbol{u}}_{int} = \frac{Z_k \boldsymbol{u}_k + Z_j \boldsymbol{u}_j}{Z_k + Z_j}
\end{cases}$$
(42)

where  $Z_k = \rho_k c_k$  and  $Z_j = \rho_j c_j$  are the impedance of the phase k and j,
respectively. The speed of sound is denoted by the variable c. The function sgn(x) returns the sign of the variable x.

The first step consists of rearranging the equations given in Eq. (42) using the
primitive variables  $(\alpha_k, \rho_k, \boldsymbol{u}_k, e_k)$ , where  $e_k$  is the specific internal energy of  $k^{th}$  phase. We introduce the material derivative  $\frac{D(\cdot)}{Dt} = \partial_t(\cdot) + \boldsymbol{u}_k \cdot \boldsymbol{\nabla}(\cdot)$  for
simplicity.

The void fraction is unchanged. The continuity equation is modified as follows:

$$\alpha_k A \frac{D\rho_k}{Dt} + \rho_k A\mu \left(P_k - P_j\right) + \rho_k A \left(\boldsymbol{u}_k - \boldsymbol{u}_j\right) \cdot \boldsymbol{\nabla} \alpha_k + \rho_k \alpha_k \boldsymbol{\nabla} \cdot (A\boldsymbol{u}_k) = 0 \quad (43)$$

The momentum and continuity equations are combined to yield the velocity equation:

$$\alpha_{k}\rho_{k}A\frac{D\boldsymbol{u}_{k}}{Dt} + \partial_{x}\left(\alpha_{k}AP_{k}\right) = \alpha_{k}P_{k}\boldsymbol{\nabla}A + P_{int}A\boldsymbol{\nabla}\alpha_{k} + A\lambda_{u}\left(\boldsymbol{u}_{j} - \boldsymbol{u}_{k}\right) \quad (44)$$

The internal energy is obtained from the total energy and the kinetic equation  $(u_k*Eq. (44))$ :

$$\alpha_{k}\rho_{k}A\frac{De_{k}}{Dt} + \nabla \cdot (\alpha_{k}\boldsymbol{u}_{k}AP_{k}) - \boldsymbol{u}_{k} \cdot \nabla (\alpha_{k}AP_{k}) = P_{int}A(\boldsymbol{u}_{int} - \boldsymbol{u}_{k}) \cdot \nabla \alpha_{k}$$
$$-\alpha_{k}P_{k}\boldsymbol{u}_{k} \cdot \nabla A - \bar{P}_{int}A\mu_{P}(P_{k} - P_{j}) + A\lambda_{u}(\boldsymbol{u}_{j} - \boldsymbol{u}_{k}) \cdot (\bar{\boldsymbol{u}}_{int} - \boldsymbol{u}_{k})$$
(45)

In the next step, we assume the existence of a phase wise entropy  $s_k$  function of the density  $\rho_k$  and the internal energy  $e_k$ . Using the chain rule,

$$\frac{Ds_k}{Dt} = (s_\rho)_k \frac{D\rho_k}{Dt} + (s_e)_k \frac{De_k}{Dt}, \tag{46}$$

along with the internal energy and the continuity equations, the following entropy equation is obtained:

$$\alpha_k \rho_k A \frac{Ds_k}{Dt} + \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} \alpha_k + \alpha_k \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(a)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot \boldsymbol{\nabla} A}_{\text{(b)}} = \underbrace{A \left( P_k(s_e)_k + \rho_k^2(s_\rho)_k \right) \boldsymbol{u}_k \cdot$$

$$(s_e)_k P_{int} A \left[ (\boldsymbol{u}_{int} - \boldsymbol{u}_k) \cdot \boldsymbol{\nabla} \alpha_k - \bar{P}_{int} A \mu_P (P_k - P_j) + A \lambda_u (\bar{\boldsymbol{u}}_{int} - \boldsymbol{u}_k) \cdot (\boldsymbol{u}_j - \boldsymbol{u}_k) \right] - \rho^2 (s_\rho)_k \left[ \mu_P A (P_k - P_j) + A (\boldsymbol{u}_k - \boldsymbol{u}_{int}) \cdot \boldsymbol{\nabla} \alpha_k \right]$$
(47)

where  $(s_e)_k$  and  $(s_\rho)_k$  denote the partial derivatives of the entropy  $s_k$  with respect to the internal energy  $e_k$  and the density  $\rho_k$ , respectively. The second term, (a), in the left hand side of Eq. (47) can be set to zero by assuming the

following relation between the partial derivatives of the entropy  $s_k$ :

$$P_k(s_e)_k + \rho_k^2(s_\rho)_k = 0. (48)$$

The above equation is equivalent to the application of the second thermodynamic law when assuming reversibility:

$$T_k ds_k = de_k - \frac{P_k}{\rho_k^2} d\rho_k \text{ with } (s_e)_k = \frac{1}{T_k} \text{ and } (s_\rho)_k = -\frac{P_k}{\rho_k^2} (s_e)_k$$
 (49)

Thus, equation Eq. (47) can be rearranged using the relation  $(s_{\rho})_k = -\frac{P_k}{\rho_L^2}(s_e)_k$ :

$$((s_e)_k)^{-1}\alpha_k\rho_k\frac{Ds}{Dt} = \underbrace{[P_{int}(\boldsymbol{u}_{int} - \boldsymbol{u}_k) + P_k(\boldsymbol{u}_k - \boldsymbol{u}_{int})] \cdot \boldsymbol{\nabla}\alpha_k}_{\text{(b)}} + \underbrace{\mu(P_k - P_j)(P_k - \bar{P}_{int})}_{\text{(c)}} + \underbrace{\lambda(\boldsymbol{u}_j - \boldsymbol{u}_k) \cdot (\bar{\boldsymbol{u}}_{int} - \boldsymbol{u}_k)}_{\text{(d)}}$$
(50)

The right hand side of equation Eq. (50) is split into three terms (b), (c) and (d) that will be treated independently from each other. The terms (c) and (d) are simpler to start with and can be easily recast by using the definitions of  $\bar{u}_{int}$  and  $\bar{P}_{int}$  given in equation Eq. (42):

$$\mu(P_k - P_j)(P_k - \bar{P}_{int}) = \mu_P \frac{Z_k}{Z_k + Z_j} (P_j - P_k)^2$$

$$\lambda(\boldsymbol{u}_j - \boldsymbol{u}_k) \cdot (\bar{\boldsymbol{u}}_{int} - \boldsymbol{u}_k) = \lambda_u \frac{Z_j}{Z_k + Z_j} (\boldsymbol{u}_j - \boldsymbol{u}_k)^2$$
(51)

By definition,  $\mu_P$ ,  $\lambda_u$  and  $Z_k$  are all positive. Thus, the above terms are unconditionally positive.

It remains to look at the last term (b). Once again, by using the definition of  $P_{int}$  and  $u_{int}$ , and the following relations:

$$u_{int} - u_k = \frac{Z_j}{Z_k + Z_j} (u_j - u_k) - \frac{\nabla \alpha_k}{||\nabla \alpha_k||} \frac{Pk - P_j}{Z_k + Z_j}$$

$$P_{int} - P_k = \frac{Z_k}{Z_k + Z_j} (P_j - P_k) - \frac{\nabla \alpha_k}{||\nabla \alpha_k||} \frac{Z_k Z_j}{Z_k + Z_j} (u_k - u_j),$$

487 (b) yields:

$$[P_{int}(\boldsymbol{u}_{int} - \boldsymbol{u}_{k}) + P_{k}(\boldsymbol{u}_{k} - \boldsymbol{u}_{int})] \cdot \boldsymbol{\nabla} \alpha_{k} = (P_{int} - P_{k})(\boldsymbol{u}_{int} - \boldsymbol{u}_{k}) \cdot \boldsymbol{\nabla} \alpha_{k} = \frac{Z_{k}}{(Z_{k} + Z_{j})^{2}} \boldsymbol{\nabla} \alpha_{k} \cdot \left[ Z_{j}(\boldsymbol{u}_{j} - \boldsymbol{u}_{k})(P_{j} - P_{k}) + \frac{\boldsymbol{\nabla} \alpha_{k}}{||\boldsymbol{\nabla} \alpha_{k}||} Z_{j}^{2}(\boldsymbol{u}_{j} - \boldsymbol{u}_{k})^{2} + \frac{\boldsymbol{\nabla} \alpha_{k}}{||\boldsymbol{\nabla} \alpha_{k}||} (P_{k} - P_{j})^{2} + \frac{\boldsymbol{\nabla} \alpha_{k} \cdot \boldsymbol{\nabla} \alpha_{k}}{||\boldsymbol{\nabla} \alpha_{k}||^{2}} (P_{k} - P_{j}) Z_{j}(\boldsymbol{u}_{k} - \boldsymbol{u}_{j}) \right] (52)$$

The above equation is factorized by  $||\nabla \alpha_k||$  and then recast under a quadratic form when noticing that  $\frac{\nabla \alpha_k \cdot \nabla \alpha_k}{||\nabla \alpha_k||^2} = 1$ , which yields:

$$[(\boldsymbol{u}_{int} - \boldsymbol{u}_k)P_{int} + (\boldsymbol{u}_k - \boldsymbol{u}_{int})P_k]\boldsymbol{\nabla}\alpha_k = ||\boldsymbol{\nabla}\alpha_k|| \frac{Z_k}{(Z_k + Z_j)^2} [Z_j(\boldsymbol{u}_j - \boldsymbol{u}_k) + \frac{\boldsymbol{\nabla}\alpha_k}{||\boldsymbol{\nabla}\alpha_k||} (P_k - P_j)]^2$$
(53)

Thus, using results from Eq. (50), Eq. (51), Eq. (52) and Eq. (53), the entropy equation obtained in [3] holds and is recalled here for convenience:

$$(s_e)_k^{-1} \alpha_k \rho_k A \frac{Ds_k}{Dt} = \mu_P \frac{Z_k}{Z_k + Z_j} (P_j - P_k)^2 + \lambda_u \frac{Z_j}{Z_k + Z_j} (\boldsymbol{u}_j - \boldsymbol{u}_k)^2$$
$$\frac{Z_k}{(Z_k + Z_j)^2} \left[ Z_j (\boldsymbol{u}_j - \boldsymbol{u}_k) + \frac{\boldsymbol{\nabla} \alpha_k}{||\boldsymbol{\nabla} \alpha_k||} (P_k - P_j) \right]^2.$$

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