

Application of the entropy viscosity method to the 1-D 7-equation Model for Two-Phase Flows

Marc O. Delchini*, Jean C. Ragusa*, Ray A. Berry†

*Department of Nuclear Engineering, Texas A&M University, †Idaho National Laboratory
delcmo@tamu.edu, jean.ragusa@tamu.edu, ray.berry@inl.gov

INTRODUCTION

In this paper, we extend the entropy viscosity method, proposed by Guermond et al. [1, 2] to the well-posed 1-D 7-equation two-phase model [3, 4]. This model is obtained by integrating the single-phase flow balance equations weighed by a characteristic function for each phase. The resulting system of equations contains non-conservative terms that describe the interaction between phases but also an equation for the volume fraction. This two-phase flow model is also known to be unconditionally hyperbolic, which is highly desirable when working with approximate Riemann solvers, and can be used for a wide range of applications. Its particularity comes from the pressure and velocity relaxation terms appearing in the volume fraction, momentum, and energy equations. When employing large values for the relaxation parameters, the two phases come to be brought in equilibrium. The 7-equation model can degenerate into the 6-equation model (same phasic pressure) [5] and the 5-equation model (same phasic velocities and pressure) [6]. The 7-equation model is currently discretized in space using *discontinuous schemes* with approximate Riemann solvers derived from the well-established approaches for single-phase flows, while using an upwind-type flux for the non-conservative terms [7, 8, 9, 10, 11].

The entropy viscosity technique is a viscous regularization technique that satisfies the entropy minimum principle; adequate dissipation terms (viscous fluxes) are added to the governing laws while ensuring the entropy minimum principle still holds. Viscosity coefficients modulate the magnitude of the added dissipation such that it is large in shock regions and vanishingly small elsewhere. The entropy viscosity coefficients are taken proportional to the entropy production while, at the same time, being bounded from above by a first-order viscosity coefficient that reduces the spatial discretization to be similar to a first-order Godunov scheme (the latter being known to be overly dissipative but monotone [12]). Hence, entropy production in shocks will result in large viscosity coefficients and thus will avoid spurious oscillations.

The entropy method is independent of the type of spatial discretization (finite volume, continuous or discontinuous finite elements, ...) and thus can be applied ubiquitously. The results presented in this summary were obtained with RELAP-7 [13], the next-generation reactor safety system code built upon the MOOSE multiphysics framework [14] that uses a *Continuous Galerkin Finite Element Method*.

In this summary, the 1-D 7-equation model is recalled along with the dissipative terms used in the entropy method. Definition of the viscosity coefficients is also given and numerical results are presented for a 1-D two-phase flow shock tube.

THEORY

We recall the 1-D 7-equation model for phase k in interaction with phase j where we have already added, for conciseness, the viscous regularization terms based on the entropy-viscosity method:

$$\frac{\partial \alpha_k A}{\partial t} + u_{int} A \frac{\partial \alpha_k}{\partial x} = A \mu_P (p_k - p_j) + \boxed{\frac{\partial}{\partial x} (A l_k)} \quad (1a)$$

$$\frac{\partial (\alpha \rho)_k A}{\partial t} + \frac{\partial (\alpha \rho u)_k A}{\partial x} = \boxed{\frac{\partial}{\partial x} (A f_k)} \quad (1b)$$

$$\begin{aligned} \frac{\partial (\alpha \rho u)_k A}{\partial t} + \frac{\partial \alpha_k A (\rho u^2 + p)_k}{\partial x} &= p_{int} A \frac{\partial \alpha_k}{\partial x} \\ &+ p_k \alpha_k \frac{\partial A}{\partial x} + A \lambda_u (u_j - u_k) \\ &+ \boxed{\frac{\partial}{\partial x} [A (g_k + u_k f_k)]} \end{aligned} \quad (1c)$$

$$\begin{aligned} \frac{\partial (\alpha \rho E)_k A}{\partial t} + \frac{\partial \alpha_k u_k A (\rho E + p)_k}{\partial x} &= p_{int} u_{int} A \frac{\partial \alpha_k}{\partial x} \\ &- \bar{p}_{int} A \mu_P (p_k - p_j) + \bar{u}_{int} A \lambda_u (u_j - u_k) \\ &+ \boxed{\frac{\partial}{\partial x} \left[A \left(h_k + u_k g_k - \frac{u_k^2}{2} f_k + \rho_k e_k l_k \right) \right]} \end{aligned} \quad (1d)$$

where the dissipative terms, boxed in Eq .1, have the following definition:

$$l_k = \beta_k \partial_x \alpha_k \quad (2a)$$

$$f_k = \alpha_k \kappa_k \partial_x \rho_k + \rho_k l_k \quad (2b)$$

$$g_k = \alpha_k \mu_k \rho_k \partial_x u_k \quad (2c)$$

$$h_k = \alpha_k \kappa_k \partial_x (\rho_k e_k) \quad (2d)$$

The notation is standard: α_k , ρ_k , $(\rho \vec{u})_k$ and $(\rho E)_k$ are the volume fraction, the density, the momentum and the total energy for phase k , respectively, and will be referred to as the conservative variables. u_k is the fluid velocity for phase k and its specific internal energy is denoted by $e_k = E_k - \frac{u_k^2}{2}$. The area A is a given and can be spatial-dependent. An equation of state is used to compute the pressure P_k . Definitions of the interfacial variables denoted by the subscript *int* can be found in [4]. As mentioned in the introduction, each viscosity coefficient is function of an upper bound referred to as the first-order viscosity and denoted by the subscript

max, and a high-order viscosity coefficient denoted by the subscript e as follows:

$$\begin{aligned}\mu_k^K(x_q, t) &= \min(\mu_{max,k}^K(x_q, t), \mu_{e,k}^K(x_q, t)), \\ \kappa_k^K(x_q, t) &= \min(\kappa_{max,k}^K(x_q, t), \kappa_{e,k}^K(x_q, t)) \\ \text{and } \beta_k^K(x_q, t) &= \min(\beta_{max,k}^K(x_q, t), \beta_{e,k}^K(x_q, t))\end{aligned}$$

where K is a given element of the mesh, and x_q is a quadrature point location within cell K . The first-order viscosity coefficients, $\mu_{max,k}^K$ and $\kappa_{max,k}^K$, are only present in the continuity, momentum and energy equations of each phase, and thus are defined proportional to the local maximum eigenvalue $u_k + c_k$.

$$\begin{aligned}\mu_{max,k}^K(x_q, t) &= \mu_{max,k}^K(x_q, t) = \frac{h^K}{2}(u_k(x_q, t) + c_k(x_q, t)) \\ \beta_{max,k}^K(x_q, t) &= \frac{h^K}{2}\|u_{int}(x_q, t)\|,\end{aligned}$$

where h^K is the grid size of element K . On the other hand, the first-order viscosity coefficient $\beta_{max,k}^K$ is defined proportional to the eigenvalue u_{int} since intimately related to the void fraction equation. The high-order viscosity coefficients, $\beta_{e,k}^K$, $\kappa_{e,k}^K$ and $\mu_{e,k}^K$ are distinct positive viscosity coefficients and are based on the local entropy production in phase k . The definition of the coefficients $\mu_{e,k}^K$ and $\kappa_{e,k}^K$ is identical to the one used for the multi-D Euler equations [15] and yield well-scaled dissipative terms in the low-Mach regime [16, 17, 18]:

$$\kappa_{e,k}^K(x_q, t) = h_K^2 \frac{\max(|\tilde{R}_k^K(x_q, t)|, J_P^K)}{\rho_k c_k^2} \quad (3a)$$

$$\mu_{e,k}^K(x_q, t) = Pr_k \kappa_{e,k}^K(x_q, t) \quad (3b)$$

where c_k is the phase speed of sound and the weighting factor is the local Mach number, $M_k = u_k/c_k$. Pr_k is the Prandtl number; see [1] for additional details. The entropy residual is denoted by R and its definition is recalled in Eq. (4).

$$\tilde{R}(\vec{r}_q, t) := \left(\frac{DP_k}{Dt} - c_k^2 \frac{D\rho_k}{Dt} \right), \quad (4)$$

where s_k is the phase entropy, function of the density ρ_k and the internal energy e_k . Proof of Eq. (4) can be found in [15]. Lastly, the quantity J_P denotes the inter element jumps of the gradient of the pressure and the density (see [15] for details).

The approach to define the viscosity coefficient $\beta_{e,k}^K$ is similar to the logic followed for hyperbolic scalar equations [1, 2]: an entropy equation can be derived from the volume fraction equation (Eq. (1a)) and used in the definition of the coefficient $\beta_{e,k}^K$. Following the work by Guermond et al. [1, 2], one obtains:

$$\beta_{e,k}^K(x_q, t) = h_K^2 \frac{\max(|R_{\alpha,k}^K(x_q, t)|, J_\alpha^K)}{\alpha_k}, \quad (5a)$$

where the entropy residual associated to the volume fraction equation, Eq. (1a), is

$$R_{\alpha,k}^K(x_q, t) = \frac{1}{2} \left(\frac{\partial \alpha_k^2}{\partial t} + u_{int} \frac{\partial \alpha_k^2}{\partial x} \right). \quad (5b)$$

and J_α^K denotes the inter element jump of the gradient of the volume fraction.

RESULTS AND ANALYSIS

The 1-D 7-equation model with viscous stabilization is discretized with *continuous* finite elements in space and BDF2 in time using RELAP-7. The resulting nonlinear system of equations at each time step is solved using a Jacobian-free Newton Krylov technique. We present one sample result for a 1-D two-phase flow shock tube of length $L = 1 \text{ m}$ and area $A = 1 \text{ m}^2$ filled with two gas phases in equilibrium (same pressure and velocity) described by the ideal gas equation of state with $\gamma_1 = 3$ and $\gamma_2 = 1.4$, with the objective of testing adequacy of our numerical stabilization method. Initially, a membrane separates the shock tube pipe in two chambers, one with a high pressure ($P_{left} = 1 \text{ MPa}$) on the left side and another one with a low pressure ($P_{right} = 0.1 \text{ MPa}$) on the right. Both phases are initially at rest. The volume fraction is set to 0.5 which means each side of the chamber contains a mixture of two phases with different equation of state parameters. The pressure and velocity relaxation coefficients are computed using the expression provided in Eq. (6).

$$\lambda_u = \frac{1}{2} \mu_P Z_1 Z_2 \text{ and } \mu_P = \frac{A_{int}}{Z_1 + Z_2} \quad (6)$$

where the interfacial area is set to a large value, $A_{int} = 10^4 \text{ m}^{-1}$, so that the two phases achieve pressure and velocity equilibrium at all time. The geometry is discretized with an uniform mesh of 500 cells and the simulation is run with a CFL of 1 until $t_{final} = 305 \mu\text{s}$. The numerical results are presented in Fig. 1 to 7. An exact solution for this shock tube test is not available but numerical results obtained with a discontinuous scheme on a moving mesh can be found in [19] and use for comparison.

As expected, the two fluids have the same pressure and velocity profiles as shown in Fig. 1 and Fig. 3, respectively. The shock is well resolved and does not display any instability. The density of phases 1 and 2 have different values but experience similar variations (shock, contact and rarefaction waves), as shown in Fig. 2. The volume fraction varies because of the pressure relaxation term (Eq. (1a)) and displays a shock wave around $x = 0.7 \text{ m}$ as shown in Fig. 4. Consequently, the viscosity coefficient β_k is peaked in the shock region and also displays a second peak of lower amplitude at the location of the contact wave. Fig. 6 and Fig. 5 show the viscosity coefficients μ_k and κ_k for phase 1 and 2, respectively: they are peaked in the shock region and also display a smaller peak in the contact wave. Overall, the numerical solution is efficiently stabilized by the entropy viscosity method and the discontinuities are well resolved.

CONCLUSIONS

We have presented an extension of the entropy viscosity method to the 1-D 7-equation two-phase model and applied it to a shock tube problem with large relaxation coefficients. The numerical results show that the stabilization method is capable of stabilizing the schemes and that the viscosity coefficients are well-scaled. This work will further contribute

to the assessment of the stabilization technique for reactor flow problems in RELAP-7.

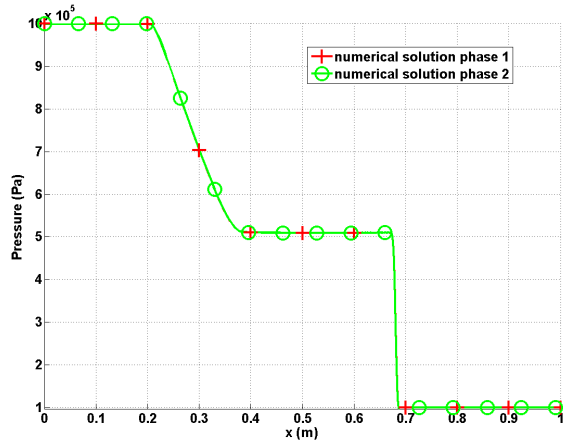


Fig. 1: Pressure at steady state.

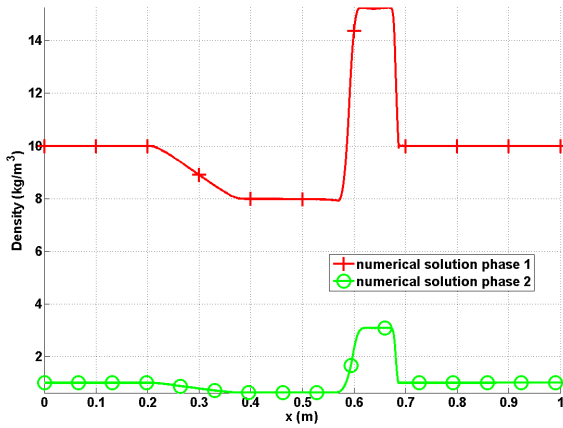


Fig. 2: Density at steady state.

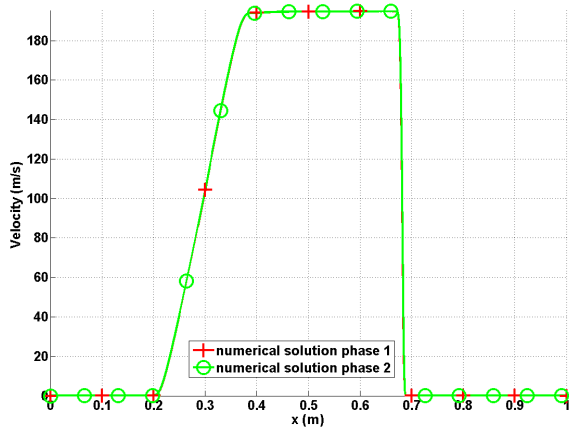


Fig. 3: Velocity at steady state.

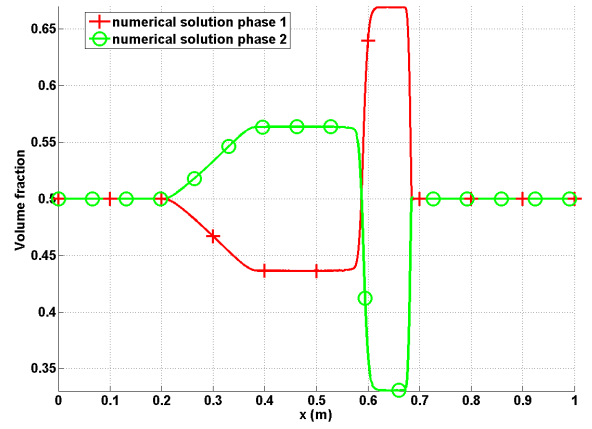


Fig. 4: Volume fraction at steady state.

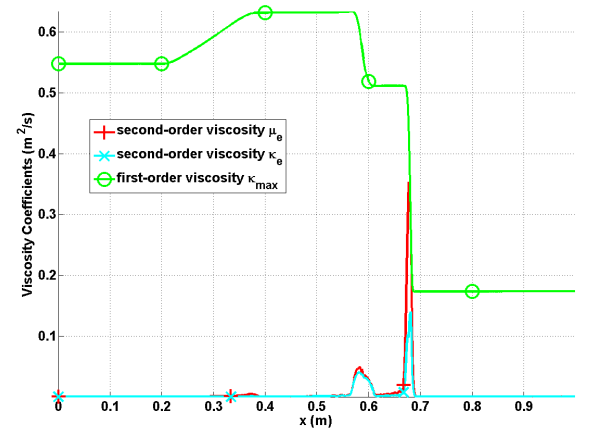


Fig. 5: Viscosity coefficients for phase 1

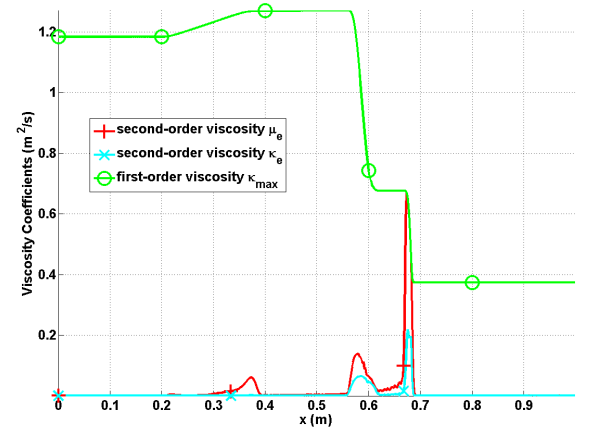


Fig. 6: Viscosity coefficients for phase 2

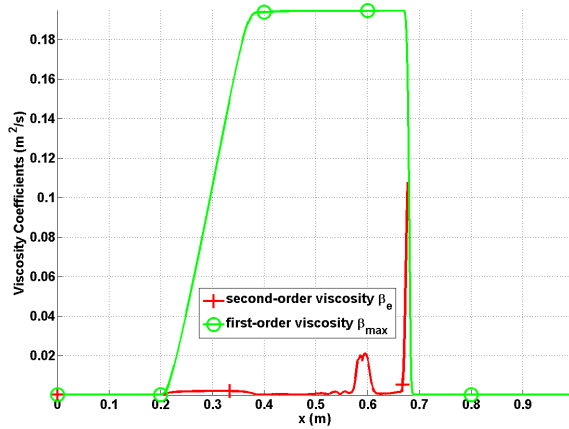


Fig. 7: Viscosity coefficients for the volume fraction.

REFERENCES

1. J. L. GUERMOND and R. PASQUETTI, "Entropy viscosity method for nonlinear conservation laws," *Journal of Comput. Phys.*, **230**, 4248–4267 (2011).
2. J. L. GUERMOND and R. PASQUETTI, "Entropy Viscosity Method for High-Order Approximations of Conservation Laws," *Lecture Notes in Computational Science and Engineering*, **76**, 411–418 (2011).
3. O. L. R. BERRY, R. SAUREL, "The discrete equation method (DEM) for fully compressible, two-phase flows in ducts of spatially varying cross-section," *Nuclear Engineering and Design*, **240**, 3797–3818 (2010).
4. R. BERRY, "A logical progression of steps for implementation and testing of the 7-equation, two-phase model into a computational framework," *International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering* (2013).
5. I. TOUMI, "An upwind numerical method for two-fluids two-phases flow models," *Nucl Sci Eng*, pp. 147–168 (1996).
6. A. K. KAPILA, R. MENIKOFF, J. B. B. S. F. SON, and D. S. STEWART, "Two-phase modeling of deflagration-to-detonation transition in granular materials," *Phys. Fluids*, pp. 3002–3024 (2001).
7. R. SAUREL and R. ABGRALL, "A multiphase Godunov method for compressible multifluid and multiphase flows," *J. Comput Physics*, pp. 425–267 (2001).
8. R. SAUREL and O. LEMETAYER, "A multiphase model for compressible flows with interfaces, shocks, detonation waves and cavitation," *J. Comput Physics*, pp. 239–271 (2001).
9. Q. LI, H. FENG, T. CAI, and C. HU, "Difference scheme for two-phase flow," *Appl Math Mech*, p. 536 (2004).
10. A. ZEIN, M. HANTKE, and G. WARNECKE, "Modeling phase transition for compressible two-phase flows applied to metastable liquids," *J. Comput Physics*, p. 2964 (2010).
11. A. AMBROSO, C. CHALONS, and P.-A. REVIART, "A Godunov-type method for the seven-equation model of compressible multiphase mixtures," *Comput. Fluids*, pp. 67–91 (2012).
12. E. F. TORO, *Riemann Solvers and numerical methods for fluid dynamics*, 2nd Edition, Springer (1999).
13. R. A. BERRY, J. W. PETERSON, H. ZHANG, R. C. MARTINEAU, H. ZHAO, L. ZOU, and D. ANDRS, "RELAP-7 Theory Manual," Tech. Rep. INL/EXT-14-31366, Idaho National Laboratory, U. S. A. (2014).
14. D. GASTON, C. NEWSMAN, G. HANSEN, and D. LEBRUN-GRANDIE, "A parallel computational framework for coupled systems of nonlinear equations," *Nucl. Eng. Design*, **239**, 1768–1778 (2009).
15. M. O. DELCHINI, J. C. RAGUSA, and R. BERRY, "Entropy-based viscous regularization for the multi-dimensional Euler equations in low-Mach and transonic flows," *under review* (2014).
16. H. GUILLARD and C. VIOZAT, "On the behavior of upwind schemes in the low Mach number limit," *Computers & Fluids*, **28**, 63–86 (1999).
17. E. TURKEL, "Preconditioned techniques in computational fluid dynamics," *Annu. Rev. Fluid Mech.*, **31**, 385–416 (1999).
18. J. S. W. D. L. DARMOFAL, and 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**, 5719–5737 (2001).
19. R. SAUREL, J. MASSONI, and F. RENAUD, "A numerical method for one-dimensional compressible multiphase flows on moving meshes," *Intern Journ for Num Methods in Fluids*, pp. 1425–1450 (2007).