## Numerical modeling of compressible two-phase flows with arbitrary-rate heat and mass transfer

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We are interested in multiphase flows with heat and mass transfer, which have applications in numerous fields of engineering, such as aerospace technologies and nuclear power plants. We describe these flows by a hyperbolic single-velocity six-equation two-phase compressible flow model [2], which is composed of the phasic mass and total energy equations, one volume fraction equation, and the mixture momentum equation:

- (1a)  $\partial_t \alpha_1 + \vec{u} \cdot \nabla \alpha_1 = \mathcal{P},$
- (1b)  $\partial_t(\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \vec{u}) = \mathcal{M},$
- (1c)  $\partial_t(\alpha_2\rho_2) + \nabla \cdot (\alpha_2\rho_2\vec{u}) = -\mathcal{M},$
- (1d)  $\partial_t(\rho \vec{u}) + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + (\alpha_1 p_1 + \alpha_2 p_2) \mathbb{I}) = 0,$

$$(1e) \qquad \partial_t(\alpha_1 E_1) + \nabla \cdot \left(\alpha_1(E_1 + p_1)\vec{u}\right) - \vec{u} \cdot \left(Y_2 \nabla(\alpha_1 p_1) - Y_1 \nabla(\alpha_2 p_2)\right) = -p_{\mathrm{I}} \mathcal{P} + \mathcal{Q} + \left(g_{\mathrm{I}} + \frac{|\vec{u}|^2}{2}\right) \mathcal{M},$$

$$(1f) \qquad \partial_t(\alpha_2 E_2) + \nabla \cdot \left(\alpha_2(E_2 + p_2)\vec{u}\right) + \vec{u} \cdot \left(Y_2 \nabla(\alpha_1 p_1) - Y_1 \nabla(\alpha_2 p_2)\right) = p_{\mathrm{I}} \mathcal{P} - \mathcal{Q} - \left(g_{\mathrm{I}} + \frac{|\vec{u}|^2}{2}\right) \mathcal{M}.$$

Above  $\alpha_k$ ,  $\rho_k$ ,  $p_k$ ,  $E_k$  denote respectively the volume fraction, density, pressure, total energy per unit volume of each phase k. Moreover,  $Y_k = \frac{\alpha_k \rho_k}{\rho}$  is the mass fraction,  $\rho = \alpha_1 \rho_1 + \alpha_2 \rho_2$  is the mixture density and  $\vec{u}$  the velocity field. The model contains source terms  $\mathcal{P}$ ,  $\mathcal{Q}$ ,  $\mathcal{M}$  accounting for volume, heat and mass transfer, respectively. These transfer terms are expressed as relaxation terms:

(2) 
$$\mathcal{P} = \mu(p_1 - p_2), \quad \mathcal{Q} = \vartheta(T_2 - T_1), \quad \mathcal{M} = \nu(g_2 - g_1),$$

where  $T_k$  denotes the phasic temperature, and  $g_k$  the phasic chemical potential.  $\mu \geq 0, \, \vartheta \geq 0, \, \nu \geq 0$  are parameters or more generally functions expressing the rate of mechanical, thermal and chemical relaxation, respectively. Here we are interested in modeling flows in mechanical equilibrium, hence we will always consider that mechanical relaxation is an instantaneous process, thus we assume  $\mu \to +\infty$ . Concerning thermal and chemical relaxation, in contrast to our previous work [2], no specific assumption is made for the heat and mass transfer rate, and hence for  $\vartheta$  and  $\nu$  (provided  $\vartheta$ ,  $\nu > 0$ ). For an accurate description of the thermodynamical processes involved in transient liquid-vapor flow problems it is often important to be able to simulate both instantaneous and finite-rate relaxation processes. For instance, in some phenomena such as fast depressurizations the delay of vaporization and the appearance of metastable states are key features in the flow dynamics [1]. In the present work we present new numerical relaxation procedures to integrate interphase transfer terms with two significant properties: the capability to describe heat and mass transfer processes with arbitrary relaxation time, and the applicability to a general equation of state. The model equations are numerically solved via a classical fractional step algorithm, where we alternate between the solution of the homogeneous hyperbolic portion of the model system via a second-order accurate HLLC/Suliciu-type finite volume scheme, and the solution of a sequence of systems of ordinary differential equations for the relaxation source terms driving the flow to mechanical, thermal and chemical equilibrium. The main idea of the novel numerical relaxation procedures is to describe relaxation processes by systems of ordinary differential equations that admit analytical semi-exact exponential solutions. This allows us to design methods that are efficient both for slow finite-rate transfers and for stiff instantaneous transfers. In particular, for instantaneous processes we show the capability of the numerical model to approximate efficiently solutions to the relaxed two-phase flow models that can be established theoretically from the parent six-equation model in the limit of instantaneous

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equilibria. Several numerical tests are then presented to show the effectiveness in modeling finite-rate heat and mass transfer, including simulations of depressurizations leading to metastable superheated liquid, and the simulation of a two-dimensional fuel injector. The latter numerical experiment is illustrated in Figure 1. In this test liquid dodecane is injected from a high-pressure tank to a chamber filled with dodecane vapor at atmospheric pressure. The Noble–Abel stiffened gas equation of state is used for the two phases. We plot results at two different times for the vapor mass fraction computed by using two different values of the chemical relaxation parameter  $\nu$ ,  $\nu=0.1$ , corresponding to a slow finite-rate process, and  $\nu\to\infty$ , corresponding to instantaneous mass transfer.

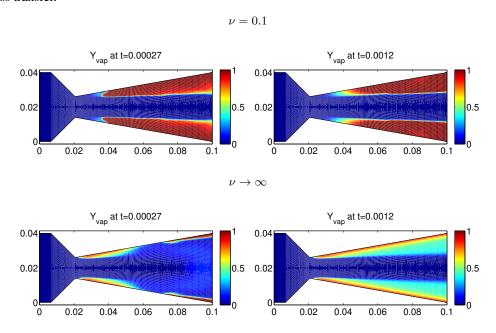


Figure 1: High-pressure fuel injector experiment. Computed vapor mass fraction  $Y_{\rm vap}$  at times  $t=0.00027,\ 0.0012\,{\rm s}$  (from left to right) for  $\nu=0.1$ , and  $\nu\to\infty$  (from top to bottom), using a  $200\times80$  grid and CFL =0.4.

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## References

- [1] M. De Lorenzo, P. Lafon, M. Di Matteo, M. Pelanti, J.-M. Seynhaeve and Y. Bartosiewicz. Homogeneous Two-Phase Flow Models and Accurate Steam-Water Table Look-up Method for Fast Transient Simulations. *Int. J. Multiphase Flow*, 95: 199–219, 2017.
- [2] M. Pelanti and K.-M. Shyue. A mixture-energy-consistent six-equation two-phase numerical model for fluids with interfaces, cavitation and evaporation waves. *J. Comput. Phys.*, 259: 331–357, 2014.
- [3] M. Pelanti. Arbitrary-rate relaxation techniques for the numerical modeling of compressible two-phase flows with heat and mass transfer. arXiv preprint arXiv:2108.00556, 2021.