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A class of compressible multiphase flow models

Une classe de modèles multiphasiques compressibles

Jean-Marc Hérard [a,b]

[a] *EDF R&D, 6, quai Watier, 78400 Chatou, France*
[b] *I2M, Aix Marseille Université, 39, rue Joliot-Curie, 13453 Marseille, France*

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A B S T R A C T

This article presents a class of barotropic multiphase models, with a hyperbolic structure, and endowed with an entropic characterization. Consistent closure laws are proposed and discussed.

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R É S U M É

On présente dans cette note une classe de modèles multiphasiques barotropes, à structure hyperbolique, et dotés d'une caractérisation entropique. Des lois de fermeture consistantes sont proposées et discutées.

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1. Introduction

The accurate modelling of multiphase flows with mixtures involving several components is crucial for several highly unsteady applications for petroleum engineering, but also for nuclear safety applications and more generally for thermal-hydraulics. Many studies in the nuclear framework, for instance those that aim at predicting hydrogen risk, vapor explosion, or similar fast transient situations, require models that comply with some basic specifications, in order to handle strong rarefaction waves as well as shock waves. Rather recent proposals have arisen within the last twenty years, at least for two-phase flow models. Some among them [1,2,5,9,10,14], which rely on the two-fluid approach, enable meaningful unsteady computations. However, only few multiphase flow models have emerged in the past in order to tackle three-phase flows or even multiphase situations. Some among the latter assume a system of PDEs for mass balance of components, while simplified momentum equations are considered (see for instance [3,7] for flows in reservoirs). More recently, a couple of contributions, among which we may cite [11,12,15,16], has given focus to the modeling of mass, momentum and energy balances for three-phase flow situations, and even more. The main objective of the present contribution is to give some new insight into this particular topic, while considering three-phase or four-phase models in order to account for unsteady compressible flows. We only consider here barotropic situations for the sake of simplicity. We first give emphasis

E-mail address: jean-marc.herard@edf.fr.

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on the modelling of interfacial transfer of momentum for multi-component flows. Next we discuss relevant closure laws for pressure and velocity relaxation terms, but also for the interface velocity that governs the evolution of statistical fractions. Finally, we give some closure laws for mass transfer.

2. A class of compressible multiphase flow models

We consider N distinct compressible phases. We also assume that the components are—at least slightly—compressible. Thus the starting point is the governing set of equations:

$$\begin{cases} \partial_t(\alpha_k) + \mathscr{V}_i(Y)\partial_x(\alpha_k) = \phi_k(Y) \,; \\ \partial_t(m_k) + \partial_x(m_k U_k) = 0 \,; \\ \partial_t(m_k U_k) + \partial_x\left(m_k U_k^2 + \alpha_k P_k(\rho_k)\right) + \Sigma_{l=1,l\neq k}^N \Pi_{kl}(Y)\partial_x(\alpha_l) = m_k S_k(Y) \,, \end{cases} \tag{1}$$

where we note $m_k = \alpha_k \rho_k$, and as usual α_k, ρ_k, U_k represent the mean statistical fraction, the mean density and the mean velocity in phase k. Mean densities are positive, and the constraint:

$$\Sigma_{k=1}^N \alpha_k = 1$$

holds everywhere, at any time. The interfacial transfer terms $\phi_k(Y)$, $S_k(Y)$ are such that:

$$\Sigma_{k=1}^N \phi_k(Y) = 0 \,; \quad \Sigma_{k=1}^N m_k S_k(Y) = 0.$$

Thus the main unknown is:

$$Y = (\alpha_1, ..., \alpha_{N-1}, \rho_1, U_1, ..., \rho_N, U_N)^t. \tag{2}$$

It lies in $\mathscr{R}^p$, with $p = 3N - 1$. The functions $P_k(\rho_k)$ are classically chosen such that $c_k^2 = P_k'(\rho_k) > 0$. We also define $\psi_k(\rho_k)$ such that:

$$\psi_k'(\rho_k) = \frac{P_k(\rho_k)}{\rho_k^2} \tag{3}$$

and the entropy of the mixture $\eta(Y)$ is defined as:

$$\eta(Y) = \frac{1}{2}\Sigma_{k=1}^N m_k U_k^2 + \Sigma_{k=1}^N m_k \psi_k(\rho_k). \tag{4}$$

From now on, we will assume that the velocity $\mathscr{V}_i(Y)$ is a convex combination of phasic velocities U_k, so that we may write:

$$\mathscr{V}_i(Y) = \Sigma_{k=1}^N a_k(Y) U_k \tag{5}$$

where $\Sigma_{k=1}^N a_k(Y) = 1$, and $0 \le a_k(Y)$.

We define the quantity $\mathscr{A}(Y, \partial_x(Y))$ such that:

$$\mathscr{A}(Y, \partial_x(Y)) = \Sigma_{k=1}^N \left(\Sigma_{l\neq k}(P_k(\mathscr{V}_i(Y) - U_k) + U_k \Pi_{kl}(Y))\partial_x(\alpha_l)\right). \tag{6}$$

Using this definition, we can obtain the governing equation of $\eta(Y)$ for smooth solutions of (1), which reads:

$$\partial_t(\eta(Y)) + \partial_x\left(f_\eta(Y)\right) = RHS_\eta(Y) - \mathscr{A}(Y, \partial_x(Y)) \tag{7}$$

setting:

$$RHS_\eta(Y) = \Sigma_{k=1}^N (m_k S_k(Y) U_k - \phi_k(Y) P_k) \tag{8}$$

$$f_\eta(Y) = \Sigma_{k=1}^N \left(\frac{U_k^2}{2} + \psi_k(\rho_k) + \frac{P_k}{\rho_k}\right) m_k U_k. \tag{9}$$

We wonder now whether there exists a unique set of $N(N-1)$ functions $\Pi_{kl}(Y)$ with $k \neq l$ that guarantees the minimal entropy dissipation $\mathscr{A}(Y, \partial_x(Y)) = 0$, when $N \le 4$.

Proposition 1 *(Closure laws for interfacial pressures). Smooth solutions of system (1) comply with the constraint $\mathscr{A}(Y, \partial_x(Y)) = 0$, iff:*

- *N=2:*

$$\Pi_{12}(Y) = \Pi_{21}(Y) = (1 - a_1(Y))P_1 + a_1(Y)P_2 \tag{10}$$

- *N=3:*

$$\begin{cases} \Pi_{12}(Y) = (1-a_1(Y))P_1 + a_1(Y)P_2 \ ; \\ \Pi_{21}(Y) = a_2(Y)P_1 + (1-a_2(Y))P_2 \ ; \\ \Pi_{13}(Y) = (1-a_1(Y))P_1 + a_1(Y)P_3 \ ; \\ \Pi_{31}(Y) = a_3(Y)P_1 + (1-a_3(Y))P_3 \ ; \\ \Pi_{23}(Y) = (1-a_2(Y))P_2 + a_2(Y)P_3 \ ; \\ \Pi_{32}(Y) = a_3(Y)P_2 + (1-a_3(Y))P_3 \ ; \end{cases} \tag{11}$$

- *N=4:*

$$\begin{cases} \Pi_{kl}(Y) = (1-a_k(Y))P_k + a_k(Y)P_l \qquad (if : 1 \leq k < l \leq 4) \ ; \\ \Pi_{kl}(Y) = a_l(Y)P_k + (1-a_l(Y))P_l \qquad (if : 1 \leq l < k \leq 4) \ . \end{cases} \tag{12}$$

Sketch of proof. The proof is obtained by construction. It is almost obvious when $N = 2$, but more tedious when $N = 3$ or $N = 4$. First it is necessary to rewrite the scalar quantity $\mathscr{A}(Y, \partial_x(Y))$ in terms of the $N-1$ independent gradients $\partial_x(\alpha_l)$ for $l = 1 \to N-1$ (since $\partial_x(\alpha_N) = -\Sigma_{l=1}^{N-1}\partial_x(\alpha_l)$). All cofactors must be set to zero, which results in a new set of $(N-1)$ scalar equations $LHS_k(Y) = 0$. For each equation among these, one must again rewrite quantities in terms of $N-1$ independent relative velocities $(U_N - U_l)$ for $l = 1 \to N-1$, and also use the form (5) in order to obtain $(U_l - \mathscr{V}_i(Y))$ in terms of the latter relative velocities and of the $a_l(Y)$. Moreover, one needs to take into account the constraint:

$$\Sigma_{k=1}^{N}\left(\Sigma_{l=1,l\neq k}^{N}\Pi_{kl}(Y)\partial_x(\alpha_l)\right) = 0$$

that arises since these represent interfacial transfer terms inside the mixture. This ends up in a system of $N(N-1)$ scalar equations, which is linear with respect to the $\Pi_{kl}(Y)$. It only remains to find the *unique* $N(N-1)$ solutions $\Pi_{kl}(Y)$ of the latter system. □

Hence, once the $a_k(Y)$ in (5) are given, there exists a unique choice for the $\Pi_{kl}(Y)$. Note that, unlike for two-phase flows, and for a given couple of phases (k,l), there exists a disequilibrium at the (k,l) interface when three (or four) phases occur, since:

$$\Pi_{kl}(Y) - \Pi_{lk}(Y) = (1 - a_k(Y) - a_l(Y))(P_k - P_l) \quad \text{for:} \quad k < l$$

is non-zero unless a perfect pressure equilibrium holds between the three (or four) phases. This was actually expected, since the quantity $\Pi_{kl}\partial_x(\alpha_l) + \Pi_{lk}\partial_x(\alpha_k)$ is no longer null, for given (k,l) with $k \neq l$, when $N > 2$. Moreover, it clearly arises that $\Pi_{kl}(Y)$ is an average of pressures P_k and P_l.

Proposition 2 *(Entropy inequality for multi-phase flow models). We consider some fixed phase index $k_0 \in 1, .., N$. We assume that closure laws for interfacial quantities $\phi_k(Y)$, $S_k(Y)$ comply with the two constraints:*

$$\begin{cases} 0 \leq \Sigma_{k=1}^{N}\left(\phi_k(Y)(P_k - P_{k_0})\right) \ ; \\ 0 \leq \Sigma_{k=1}^{N}\left(m_k S_k(Y)(U_{k_0} - U_k)\right) \end{cases} \tag{13}$$

then smooth solutions of system (1) satisfy the following inequality:

$$\partial_t(\eta(Y)) + \partial_x\left(f_\eta(Y)\right) \leq 0 \tag{14}$$

for the minimal entropy dissipation model associated with: $\mathscr{A}(Y, \partial_x(Y)) = 0$.

The proof is straightforward. We may now give some admissible form for the pressure relaxation terms.

Proposition 3 *(Pressure–velocity relaxation terms for multi-phase flow models). Assume that closure laws for $\phi_k(Y)$, $S_k(Y)$ take the form:*

$$\begin{cases} \phi_k(Y) = \Sigma_{l=1}^{N}\left(d_{kl}(Y)(P_k - P_l)\right) \ ; \\ m_k S_k(Y) = \Sigma_{l=1}^{N}\left(e_{kl}(Y)(U_l - U_k)\right) \end{cases} \tag{15}$$

with: $0 < d_{kl}(Y) = d_{lk}(Y)$, and: $0 \leq e_{kl}(Y) = e_{lk}(Y)$, then the pressure-velocity relaxation terms $\phi_k(Y)$, $S_k(Y)$ comply with the entropy inequality (14).

Proof. It is classical for $N = 2$. We skip the case $N = 3$, and we only consider here the case $N = 4$. We define: $x = P_1 - P_2$, $y = P_1 - P_3$, $z = P_1 - P_4$. The remaining pressure desequilibria may be written as follows: $P_4 - P_3 = y - z$, $P_4 - P_2 = x - z$, $P_3 - P_2 = x - y$. Hence we may compute:

$$\sigma_4 = \Sigma_{k=1}^{4} \left(\phi_k(Y)(P_k - P_1)\right)$$

which turns to be:

$$\sigma_4 = d_{21}(Y)x^2 + d_{31}(Y)y^2 + d_{41}(Y)z^2 + d_{42}(Y)(z-x)^2 + d_{32}(Y)(y-x)^2 + d_{43}(Y)(y-z)^2.$$

Thus σ_4 is strictly positive unless $P_1 = P_2 = P_3 = P_4$. □

A similar proof holds for velocity relaxation contributions. We emphasize first that the counterpart of properties 2, 3 also holds for non-isentropic two- or three-phase flow models (see [5,12,15]). Quantities $S_k(Y)$ stand for drag effects between phases; besides, pressure relaxation terms $\phi_k(Y)$ are already present in all standard two-phase flow models such as those described in [1,14], for instance. Physically relevant pressure relaxation time scales associated with the d_{kl} were proposed in [8]. One may nonetheless wonder whether these relaxation terms act as expected. Actually, the following result clearly provides some assessment of the latter claim. For that purpose, we consider some flow in a box (thus neglecting all convective effects), so that system (1) reduces to:

$$\begin{cases} \partial_t(\alpha_k) = \phi_k(Y)\,; \\ \partial_t(m_k) = 0\,; \\ \partial_t(m_k U_k) = m_k S_k(Y)\,. \end{cases} \tag{16}$$

Proposition 4 *(Pressure relaxation for barotropic three-phase flow models). We set: $N = 3$, and we assume for sake of simplicity that pressure relaxation time scales are equal, so that: $\phi_k(Y) = d(Y)\Sigma_{l=1}^{N}(P_k - P_l)$. We also define:*

$$\mathscr{E}_P(Y) = ((P_1 - P_2)^2 + (P_1 - P_3)^2 + (P_2 - P_3)^2)/2.$$

Then solutions of (16) comply with:

$$0 \le \mathscr{E}_P(Y)(t) \le \mathscr{E}_P(Y)(0) \times \exp\left(-6\int_0^t f_{\min}^P(t)\mathrm{d}t\right)$$

if the frequency $0 < f_{\min}^P(t)$ denotes some positive lower bound of $(\rho_k c_k^2 d(Y)/\alpha_k)(t)$ (for $k = 1, 3$).

Proof. We define: $y = P_1 - P_2$ and: $x = P_2 - P_3$, thus: $P_1 - P_3 = y + x$, and: $\mathscr{E}_P(Y) = x^2 + y^2 + xy$. We use the notation: $\beta_k = \rho_k c_k^2/\alpha_k$. Using the second equation of (16), which gives: $\partial_t(\rho_k) = -\rho_k\partial_t(\alpha_k)/\alpha_k$, and hence: $\partial_t(P_k) = -\rho_k c_k^2 \partial_t(\alpha_k)/\alpha_k$, it clearly arises that the solutions to (16) agree with:

$$\partial_t(x) = -\beta_2\partial_t(\alpha_2) + \beta_3\partial_t(\alpha_3)$$

$$\partial_t(y) = -\beta_1\partial_t(\alpha_1) + \beta_2\partial_t(\alpha_2)\,.$$

Since $\partial_t(\alpha_k) = 2d(Y)(P_k - \overline{P}_{lm})$, with: $\overline{P}_{lm} = (P_l + P_m)/2$, for k, l, m non-equal in $\{1,2,3\}^3$, we get at once:

$$\partial_t(\mathscr{E}_P(Y)) = -d(Y)\left(\beta_2(x-y)^2 + \beta_3(2x+y)^2 + \beta_1(x+2y)^2\right)$$

which yields:

$$\partial_t(\mathscr{E}_P(Y)) \le -f_{\min}^P(t)\left((x-y)^2 + (2x+y)^2 + (x+2y)^2\right)$$

or alternatively:

$$\partial_t(\mathscr{E}_P(Y)) \le -6 f_{min}^P(t)\mathscr{E}_P(Y)(t)$$

which ends up with the above statement. □

This property is still valid for four-phase flow models (see [13]). Considering the same assumption of a flow in a box (16), a similar property may be obtained for velocity relaxation effects in three-phase flow models, considering the counterpart of $\mathscr{E}_P(Y)$:

$$\mathscr{E}_U(Y) = ((U_1 - U_2)^2 + (U_1 - U_3)^2 + (U_2 - U_3)^2)/2.$$

It now remains to select admissible closure laws for the interface velocity $\mathscr{V}_i(Y)$, which governs the statistical fractions evolution. The specifications that are enforced here correspond to the fact that the α_l should be perfectly advected (if all phase pressures were in equilibrium), and thus without any thickening; as a consequence, one must enforce that the field associated with the eigenvalue $\lambda = \mathscr{V}_i(Y)$ should be linearly degenerated. The next proposition illustrates that feature, and it is indeed a well-known result for two-phase flow models (see [4] and [5] for instance, for barotropic and non-isentropic models, respectively, and also [6] for some generalization):

Proposition 5 *(Admissible interface velocity in barotropic three-phase flow models). We set: $N = 3$, and we still assume that: $\mathcal{V}_i(Y) = \Sigma_{k=1}^{N} a_k(Y)U_k$, with: $\Sigma_{k=1}^{N} a_k(Y) = 1$. We set: $a_k(Y) = m_k/M$ where: $M = \Sigma_{k=1}^{N} m_k$. Then the field associated with: $\lambda_{1,2} = \mathcal{V}_i(Y)$ is linearly degenerated.*

Proof. It is straightforward but cumbersome. We define $r_1(Y)$, $r_2(Y)$ the two right eigenvectors associated with the eigenvalue: $\lambda = \mathcal{V}_i(Y)$, it then only remains to check that: $\nabla_Y \lambda_{1,2}(Y) \cdot r_1(Y) = \nabla_Y \lambda_{1,2}(Y) \cdot r_2(Y) = 0$. □

A similar result holds for four-phase flow models. The structure of the contact wave associated with $\lambda = \mathcal{V}_i(Y)$ is examined in detail in [13] for $N = 3$ and $N = 4$. Actually the connection of states through the latter wave is very similar to what happens in two-phase flow models (see [4,5]). Eventually, we may give the expected result, that is:

Proposition 6 *(Structure of the convective part of system (1)). We assume that: $|U_k - \mathcal{V}_i(Y)|/c_k \neq 1$. Then system (1) is hyperbolic, since all eigenvalues are real, and the set of right eigenvectors spans the whole space of states $\mathcal{R}^p$.*

3. Taking mass transfer into account

We consider now the following system for a mixture of N phases with possible mass transfer between phases. This reads:

$$\begin{cases} \partial_t(\alpha_k) + \mathcal{V}_i(Y)\partial_x(\alpha_k) = \phi_k(Y) \,; \\ \partial_t(m_k) + \partial_x(m_k U_k) = \Sigma_{l=1, l\neq k}^{N} \Gamma_{kl}(Y) = G_k(Y) \,; \\ \partial_t(m_k U_k) + \partial_x\left(m_k U_k^2 + \alpha_k P_k(\rho_k)\right) + \Sigma_{l=1, l\neq k}^{N} \Pi_{kl}(Y)\partial_x(\alpha_l) = m_k S_k(Y) + S_k^G(Y) \,, \end{cases} \tag{17}$$

with:

$$S_k^G(Y) = \Sigma_{l=1, l\neq k}^{N} \mathcal{V}_{kl}(Y)\Gamma_{kl}(Y)$$

and: $\Gamma_{kl}(Y) + \Gamma_{lk}(Y) = 0$. We also enforce the law:

$$\mathcal{V}_{kl}(Y) = \beta_{kl}(Y)U_k + (1 - \beta_{kl}(Y))U_l,$$

with: $\beta_{kl}(Y) \in [0, 1]$. We evenmore assume symmetry, that is: $\mathcal{V}_{kl}(Y) = \mathcal{V}_{lk}(Y)$, which means that: $\beta_{kl}(Y) + \beta_{lk}(Y) = 1$. The term $\Gamma_{kl}(Y)$ simply denotes the interfacial mass transfer between phases k and l. Of course, we still consider the previous closure laws for $\phi_k(Y)$, $S_k(Y)$ and $\Pi_{kl}(Y)$.

The time evolution of the entropy η is now governed by:

$$\partial_t(\eta(Y)) + \partial_x\left(f_\eta(Y)\right) = RHS_\eta^G(Y) \tag{18}$$

but the source term on the right handside becomes:

$$\begin{aligned} RHS_\eta^G(Y) &= \Sigma_{k=1}^{N}(m_k S_k(Y)U_k - \phi_k(Y)P_k) \\ &\quad + \Sigma_{k=1}^{N}\left(U_k(\Sigma_{l=1, l\neq k}^{N}\mathcal{V}_{kl}(Y)\Gamma_{kl}(Y) - \frac{U_k}{2}G_k(Y)) + G_k(Y)(\frac{P_k}{\rho_k} + \psi_k(\rho_k))\right). \end{aligned} \tag{19}$$

Thus we get the following proposition.

Proposition 7 *(An entropy-consistent closure law for the interfacial mass transfer). Assume that: $\beta_{kl}(Y) = 1/2$, and also that $f_{kl}(Y) = f_{lk}(Y) > 0$. Then the following closure law for the mass transfer:*

$$\Gamma_{kl}(Y) = f_{kl}(Y)\left((\frac{P_l}{\rho_l} + \psi_l(\rho_l)) - (\frac{P_k}{\rho_k} + \psi_k(\rho_k))\right) \tag{20}$$

complies with the entropy inequality for smooth solutions Y of (17):

$$\partial_t(\eta(Y)) + \partial_x\left(f_\eta(Y)\right) \leq 0. \tag{21}$$

The proof is simple and left to the reader, who is referred to [13]. The latter reference also provides more details and a thorough analysis of the statistical fraction LD wave $\lambda = \mathcal{V}_i(Y)$. Details on (unique) jump conditions can also be found therein. The extension to the framework of non-isentropic multiphase multi-component flows is currently investigated for $4 \leq N$.

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