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Numerical Analysis

A hyperbolic three-phase flow model

Jean-Marc Hérard^{a,b}

^a Département M.F.E.E., E.D.F., Recherche et Développement, 6, quai Watier, 78401 Chatou cedex, France ^b L.A.T.P. (UMR CNRS 6632), C.M.I., université Aix-Marseille I, 39, rue Joliot Curie, 13453 Marseille cedex 13, France

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Abstract

We introduce a hyperbolic entropy-consistent model to describe three-phase flows, which ensures that void fractions, mass fractions and pressures remain positive through single waves occurring in the one dimensional solution of the Riemann problem. *To cite this article: J.-M. Hérard, C. R. Acad. Sci. Paris, Ser. I* 342 (2006).

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Résumé

Un modèle hyperbolique d'écoulement triphasique. On introduit un modèle hyperbolique pour la modélisation des écoulements triphasiques, qui est muni d'une inégalité d'entropie physique et assure la positivité des fractions volumiques, des densités et énergies internes dans les ondes simples apparaissant dans le problème de Riemann unidimensionnel. *Pour citer cet article : J.-M. Hérard, C. R. Acad. Sci. Paris, Ser. I 342 (2006).*

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Version française abrégée

On propose ici un modèle hyperbolique sur l'ensemble des états admissibles, admettant une inégalité d'entropie physiquement admissible, et permettant d'effectuer des simulations d'écoulements triphasiques. Plusieurs modèles hyperboliques ont été proposés dans la littérature récente, qui permettent de simuler des écoulements instationnaires diphasiques, notamment dans [1,7,13,12,14,17]. Néanmoins, dans certaines configurations industrielles, il est nécessaire de considérer la présence de trois phases, et dans le domaine nucléaire, on est parfois amené à envisager une modélisation analogue dite à trois champs [18]. La littérature propose pour les écoulements en milieu poreux des modèles triphasiques basés sur la simulation de trois équations de bilan de masse, les vitesses phasiques étant modélisés à l'aide de lois de type Darcy, les écarts de pression entre phases (pressions capillaires) étant représentés par des fonctions des variables de saturation (voir par exemple [9,10,5]). La variable d'état de ces systèmes est constituée de deux saturations et d'une pression. La différence essentielle ici réside dans le fait que l'on veut décrire les évolutions des débits massiques et des énergies totales par des équations aux dérivées partielles. Le modèle, qui doit prendre en compte les effets de transfert interfacial de quantité de mouvement et d'énergie et autoriser la simulation de phénomènes instationnaires, comporte onze équations d'évolution.

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E-mail address: jean-marc.herard@edf.fr (J.-M. Hérard).

On présente tout d'abord une classe de modèles hyperboliques sans condition ayant une forme symètrique (1)-(4), (6), (7). Cette classe fait intervenir une vitesse interfaciale V_i ($V_i = \beta_1 U_1 + \beta_2 U_2 + \beta_3 U_3$, avec $\beta_1 + \beta_2 + \beta_3 = 1$), et six fonctions P_{kl} ($k \neq l$) intervenant dans le transfert interfacial de quantité de mouvement et d'énergie, qui sont liées par (5). On se concentre ensuite sur un de ces modèles qui s'apparente au modèle non symétrique de Baer et Nunziato [1,17], et correspond au choix $V_i = U_1$ (la phase 1 est diluée) associé à (8). Si les termes sources de trainée statique et les termes de relaxation en pression vérifient les conditions (9), (10) le système global est alors muni d'une inégalité d'entropie (11) valable pour les solutions régulières. Pour de telles solutions, le principe du maximum pour les taux de présence est vérifié. En outre, si chaque phase est munie d'une loi de type gaz parfait, les pressions phasiques restent positives, ainsi que les densités partielles, modulo des conditions classiques portant sur les champs de vitesse. Ce résultat reste valable lorsqu'on analyse les ondes simples isolées, dans une perspective de résolution du problème de Riemann unidimensionnel sous jacent. Cette propriété est intimement liée au fait que le champ associé à la valeur propre V_i est linéairement dégénéré d'une part, et à la forme des tranferts interfaciaux de quantité de mouvement et d'énergie totale phasique d'autre part. On est en effet ainsi en mesure de donner un sens aux produits non conservatifs sous jacents, tout comme dans le cadre diphasique (voir [7]). Les lois de fermeture des transferts interfaciaux de quantité de mouvement proposés dans [18] par exemple, permettent de satisfaire la condition (9). Le modèle considéré, muni de ses lois de fermeture, autorise ainsi la simulation d'écoulements triphasiques, en considérant indifféremment des schémas simples tels que le schéma de Rusanov, ou un schéma de Godunov approché tel que ceux décrits dans [3]. Il est indéniable que le nombre d'ondes présentes dans le système convectif nécessite l'utilisation de schémas précis et de maillages très fins, si l'on souhaite effectuer une approximation raisonnable des solutions du système considéré. Cette remarque vaut d'autant plus que le système comporte trois champs linéairement dégénérés distincts associés à des valeurs propres de module faible devant celui afférent aux ondes « rapides ». Tout comme dans le cadre diphasique [16], il est également possible, en ayant recours aux techniques de relaxation [2,4,8] et en utilisant par exemple un schéma pour l'étape de relaxation semblable à celui introduit dans [6], de simuler sur maillage grossier le modèle avec relaxation instantanée en pression semblable à celui de [18]. Il est a priori possible de prendre en compte des modèles de turbulence statistique élémentaires avec fermeture en un point, sans remettre en cause le domaine d'hyperbolicité. Dans ce cas néanmoins, le problème de fermeture des relations de saut pour la variable d'énergie cinétique turbulente phasique dans les champs vraiment non linéaires reste conjectural. On renvoie le lecteur à [15] pour plus de détails sur les propriétés du modèle, sa mise en oeuvre numérique par technique de type Volumes Finis, et des formes des termes sources de transfert de masse et d'énergie compatibles avec l'inégalité d'entropie.

1. Introduction

Some applications in the nuclear power energy and petroleum engineering require modelling of three phase flows, either in a one dimensional or in a three dimensional framework. In order to compute unsteady flows in an expected meaningful way, and especially when one aims at predicting phenomena such as the boiling crisis, or the loss of primary coolant accidents, or any other severe situation, one needs to handle well posed initial value problems. Since single pressure models may fail in many situations, when one refines the mesh size [16], owing to the loss of hyperbolicity, we propose herein a class of hyperbolic models to deal with this kind of flows. The basic ideas rely on the counterpart of the two-phase two-pressure formalism which is now quite well-known [1,7,11,13,12,14,17]. One of the main difficulties here is to define correct interfacial transfer terms, in such a way that for physically relevant initial conditions, smooth solutions but also discontinuous solutions are correctly defined, and remain in their physical domain. Another goal consists in getting a physically admissible entropy condition to keep the whole under control. An – obviously compulsory – underlying assumption in the model is that the interface should remain thin in the convective process, as already mentioned in [7] for instance. This corresponds to the fact that the field associated with the eigenvalue V_i should be linearly degenerated. Though some non-conservative terms are present in the system, the internal structure of fields will be such that non-conservative products are well defined.

2. A class of hyperbolic models

We first present here a general class of *hyperbolic* models which is symmetric with respect to the phase index. We will focus in the next section on a particular model that belongs to this class. The density, velocity, pressure, internal energy and total energy within phase k will be denoted ρ_k , U_k , P_k , $e_k = e_k(P_k, \rho_k)$ and $E_k = 0.5\rho_k U_k U_k + \rho_k e_k$

respectively, and the volumetric fraction of phase labelled k is defined as α_k . Setting $m_k = \alpha_k \rho_k$, the state variable W which lies in \mathbb{R}^{11} is:

$$W^{t} = (\alpha_{2}, \alpha_{3}, m_{1}, m_{2}, m_{3}, m_{1}U_{1}, m_{2}U_{2}, m_{3}U_{3}, \alpha_{1}E_{1}, \alpha_{2}E_{2}, \alpha_{3}E_{3}).$$
(1)

A model for the interface velocity denoted V_i will be required. We also need to introduce scalar functions $\phi_k(W)$ and momentum interfacial transfer terms S_{U_k} (for k = 1, 2, 3) which must comply with the constraints:

$$\sum_{k=1}^{3} \alpha_k = 1; \quad \sum_{k=1}^{3} \phi_k(W) = 0; \quad \sum_{k=1}^{3} S_{U_k}(W) = 0.$$
(2)

Using an initial condition $W(x, 0) = W_0(x)$ and suitable boundary conditions, the governing set of equations is:

$$\left(I + D(W)\right)\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial G(W)}{\partial x} = S(W) + \frac{\partial}{\partial x}\left(E(W)\frac{\partial W}{\partial x}\right).$$
(3)

The fluxes F(W), G(W) and the source terms S(W) lie in \mathbb{R}^{11} .

$$F(W)^{t} = (0, 0, m_{1}U_{1}, m_{2}U_{2}, m_{3}U_{3}, \alpha_{1}(\rho_{1}U_{1}^{2} + P_{1}), \alpha_{2}(\rho_{2}U_{2}^{2} + P_{2}), \alpha_{3}(\rho_{3}U_{3}^{2} + P_{3}), \\ \alpha_{1}U_{1}(E_{1} + P_{1}), \alpha_{2}U_{2}(E_{2} + P_{2}), \alpha_{3}U_{3}(E_{3} + P_{3})).$$

Second rank tensors C(W), D(W), E(W) lie in $\mathbb{R}^{11 \times 11}$. The non-conservative convective terms are:

$$\begin{cases} D(W)\frac{\partial W}{\partial t} = \left(0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -\sum_{l=1, l\neq 1}^{3} P_{ll}\frac{\partial \alpha_l}{\partial t}, -\sum_{l=1, l\neq 2}^{3} P_{2l}\frac{\partial \alpha_l}{\partial t}, -\sum_{l=1, l\neq 3}^{3} P_{3l}\frac{\partial \alpha_l}{\partial t}\right);\\ C(W)\frac{\partial G(W)}{\partial x} = \left(V_l\frac{\partial \alpha_2}{\partial x}, V_l\frac{\partial \alpha_3}{\partial x}, 0, 0, 0, \sum_{l=1, l\neq 1}^{3} P_{1l}\frac{\partial \alpha_l}{\partial x}, \sum_{l=1, l\neq 2}^{3} P_{2l}\frac{\partial \alpha_l}{\partial x}, \sum_{l=1, l\neq 3}^{3} P_{3l}\frac{\partial \alpha_l}{\partial x}, 0, 0, 0\right) \end{cases}$$
(4)

and contribute to the interfacial transfer if the six unknowns P_{kl} obey the two constraints:

$$P_{12} + P_{32} = P_{13} + P_{23} = P_{21} + P_{31}.$$
(5)

Viscous terms should at least account for the following contributions (thermal fluxes might be included):

$$E(W)\frac{\partial W}{\partial x} = \left(0, 0, 0, 0, 0, \alpha_1 \mu_1 \frac{\partial U_1}{\partial x}, \alpha_2 \mu_2 \frac{\partial U_2}{\partial x}, \alpha_3 \mu_3 \frac{\partial U_3}{\partial x}, \alpha_1 \mu_1 U_1 \frac{\partial U_1}{\partial x}, \alpha_2 \mu_2 U_2 \frac{\partial U_2}{\partial x}, \alpha_3 \mu_3 U_3 \frac{\partial U_3}{\partial x}\right).$$
(6)

Source terms S(W) account for mass transfer terms, drag effects, energy loss, and other contributions. To simplify our presentation, we only retain here the effect of pressure relaxation and drag effects. Thus:

$$S(W) = (\phi_2, \phi_3, 0, 0, 0, S_{U_1}, S_{U_2}, S_{U_3}, V_i S_{U_1}, V_i S_{U_2}, V_i S_{U_3}).$$
⁽⁷⁾

3. Main properties of a particular three-phase flow model

We now focus on the counterpart of the asymmetric Baer–Nunziato model (other choices – including the symmetric case $V_i = (\sum_k m_k U_k)/(\sum_k m_k)$ discussed in [7,11] – can be found in [15], Appendix G, which provides a unique set of unknowns P_{kl} in terms of V_i), and thus consider the particular choice $V_i = U_1$ together with:

$$P_{13} = P_{31} = P_{32} = P_3;$$
 $P_{12} = P_{21} = P_{23} = P_2.$ (8)

This for instance will correspond to the situation where the phase labelled 1 is dilute. We focus first on the homogeneous problem associated with the left-hand side of (3). We define as usual specific entropies s_k and speeds c_k in terms of the density ρ_k and the internal energy e_k :

$$(c_k)^2 = \frac{\gamma_k P_k}{\rho_k} = \left(\frac{P_k}{(\rho_k)^2} - \frac{\partial e_k(P_k, \rho_k)}{\partial \rho_k}\right) \left(\frac{\partial e_k(P_k, \rho_k)}{\partial P_k}\right)^{-1};$$

$$\gamma_k P_k \frac{\partial s_k(P_k, \rho_k)}{\partial P_k} + \rho_k \frac{\partial s_k(P_k, \rho_k)}{\partial \rho_k} = 0.$$

Property 1: The homogeneous system associated with the left-hand side of (3) has real eigenvalues: $\lambda_{1,2,3} = U_1$, $\lambda_4 = U_2$, $\lambda_5 = U_3$, $\lambda_6 = U_1 - c_1$, $\lambda_7 = U_1 + c_1$, $\lambda_8 = U_2 - c_2$, $\lambda_9 = U_2 + c_2$, $\lambda_{10} = U_3 - c_3$, $\lambda_{11} = U_3 + c_3$. Associated right eigenvectors span the whole space \mathbb{R}^{11} unless $|U_1 - U_k| = c_k$, for k = 2, 3. Fields associated with eigenvalues λ_k with k in 1, 5 are Linearly Degenerated; other fields are Genuinely Non Linear.

Riemann invariants through LD fields associated with k = 4, 5 and GNL fields may be computed quite easily (see [15]). Moreover:

Property 2: 2.1. The latter system admits the following Riemann invariants through the 1–2–3 LD wave:

$$I_1^{1-2-3}(W) = m_2(U_2 - U_1); \qquad I_2^{1-2-3}(W) = m_3(U_3 - U_1);$$

$$I_3^{1-2-3}(W) = s_2; \qquad I_4^{1-2-3}(W) = s_3; \qquad I_5^{1-2-3}(W) = U_1;$$

$$I_6^{1-2-3}(W) = \alpha_1 P_1 + \alpha_2 P_2 + \alpha_3 P_3 + m_2(U_1 - U_2)^2 + m_3(U_1 - U_3)^2;$$

$$I_7^{1-2-3}(W) = 2e_2 + 2\frac{P_2}{\rho_2} + (U_1 - U_2)^2; \qquad I_8^{1-2-3}(W) = 2e_3 + 2\frac{P_3}{\rho_3} + (U_1 - U_3)^2.$$

2.2. We note $\Delta(\psi) = \psi_r - \psi_l$. Apart from the 1–2–3 LD wave, the following exact jump conditions hold for k = 1, 2, 3, through any discontinuity separating states l, r moving with speed σ :

$$\Delta(\alpha_k) = 0; \qquad \Delta(m_k(U_k - \sigma)) = 0; \\ \Delta(m_k U_k(U_k - \sigma) + \alpha_k P_k) = 0; \qquad \Delta(\alpha_k E_k(U_k - \sigma) + \alpha_k P_k U_k) = 0.$$

We also need to define: $a_k = (s_k)^{-1} \left(\frac{\partial s_k(P_k,\rho_k)}{\partial P_k}\right) \left(\frac{\partial e_k(P_k,\rho_k)}{\partial P_k}\right)^{-1}$, and we introduce: $\eta_k = \text{Log}(s_k)$, and the pair (η, F_η) such that: $\eta = -m_1\eta_1 - m_2\eta_2 - m_3\eta_3$ and $F_\eta = -m_1\eta_1U_1 - m_2\eta_2U_2 - m_3\eta_3U_3$. We assume in addition that drag terms $S_{U_k}(W)$ and source terms $\phi_k(W)$ in (3) comply with:

$$0 \leq a_2(U_1 - U_2)S_{U_2}(W) + a_3(U_1 - U_3)S_{U_3}(W);$$
(9)

$$0 \leqslant a_1(\phi_1 P_1 + \phi_2 P_2 + \phi_3 P_3). \tag{10}$$

Condition (10) reads: $\phi_2(P_1 - P_2) + \phi_3(P_1 - P_3) \le 0$ since $\phi_1 + \phi_2 + \phi_3 = 0$ and $a_1 > 0$ for standard EOS.

Property 3: Closures in agreement with constraints (9), (10) ensure that the following entropy inequality holds for regular solutions of (3):

$$\frac{\partial \eta}{\partial t} + \frac{\partial F_{\eta}}{\partial x} \leqslant 0. \tag{11}$$

We from now will assume that the conditions (9), (10) are fulfilled. For convenience we will choose here:

$$\begin{split} \phi_2 &= f_{1-2}(W)\alpha_1\alpha_2(P_2-P_1)/(P_1+P_2+P_3) + f_{2-3}(W)\alpha_2\alpha_3(P_2-P_3)/(P_1+P_2+P_3); \\ \phi_3 &= f_{1-3}(W)\alpha_1\alpha_3(P_3-P_1)/(P_1+P_2+P_3) + f_{2-3}(W)\alpha_2\alpha_3(P_3-P_2)/(P_1+P_2+P_3). \end{split}$$

The three positive scalar functions $f_{k-l}(W)$ denote frequencies which should remain bounded over $\Omega \times [0, T]$. It is easy to check that $\phi_1 P_1 + \phi_2 P_2 + \phi_3 P_3 = (P_1 + P_2 + P_3)^{-1} (\sum_{k < l} f_{k-l}(W) \alpha_k \alpha_l (P_l - P_k)^2) > 0$. Moreover, we get: $\frac{\partial \pi}{\partial t} + U_1 \frac{\partial \pi}{\partial x} = \pi (\sum_{k < l} f_{k-l}(W) (\alpha_k - \alpha_l) (P_l - P_k)) (P_1 + P_2 + P_3)^{-1}$, when defining $\pi = \alpha_1 \alpha_2 \alpha_3$. This guarantees that regular solutions $\alpha_k(x, t)$ will remain in the admissible range [0, 1] over $\Omega \times [0, T]$. This is the straightforward counterpart of the closure law in two-phase flow models (see references herein). Moreover, we will rely on standard closures of the form (see [18] for instance): $S_{U_k}(W) = \psi_k(W)(U_1 - U_k)$ (for k = 2, 3), where the scalar functions $\psi_2(W), \psi_3(W)$ should remain positive. Hence (9) and (10) hold.

Property 4: We assume perfect gas state law within each phase (k = 1, 2, 3). We consider a single wave associated with λ_m , separating states l, r. If the initial conditions satisfy: $(\alpha_k)_{L,R}(1 - \alpha_k)_{L,R} \neq 0$, for k = 1, 2, 3 the connection of states through this wave ensures that all states are in agreement with: $0 \leq \alpha_k, 0 \leq m_k, 0 \leq P_k$.

Actually, the proof is almost obvious when focusing on a single field connected with eigenvalue λ_k where k = 4 to 11. Turning then to the 1, 2, 3-field, the main guidelines are almost the same as in [11] (see [15]). The whole enables to introduce a fractional step approach in agreement with the overall entropy inequality, which is again the counterpart of the one described in [11]. Owing to the entropy structure, one may even use the pressure relaxation step as a tool to compute the single pressure models detailed in [18] on coarse meshes, as may be done in



the two-phase framework (see [16] for instance). The connection with the early scheme introduced in [6] is obvious. In order to compute convective terms, one may apply the approximate Godunov scheme [3] with the variable $Z^t = (\alpha_2, \alpha_3, s_1, s_2, s_3, U_1, U_2, U_3, P_1, P_2, P_3)$. Some suitable forms of mass transfer terms can be found in [15]. We eventually provide some computational results. We assume that the perfect gas law holds within each phase: $\rho_k e_k (\gamma_k - 1) = P_k$, setting $\gamma_1 = 7/5$, $\gamma_2 = 1.05$ and $\gamma_3 = 1.01$. In this example, phase 1 refers to the gas phase, and the other two correspond to two distinct liquids. Setting $Y^t = (\alpha_2, \alpha_3, U_1, \tau_1, P_1, U_2, \tau_2, P_2, U_3, \tau_3, P_3)$, initial conditions are:

$$Y_L = (0.4, 0.5, 10^2, 1, 10^5, 10^2, 1, 10^5, 10^2, 1, 10^5)$$
 and $Y_R = (0.5, 0.4, 10^2, 8, 10^5, 10^2, 8, 10^5, 10^2, 8, 10^5)$

for the first case (Figs. 1–3), while we choose for the second test (Figs. 4–6):

 $Y_L = (0.4, 0.5, 0, 1, 10^5, 0, 1, 10^5, 0, 1, 10^5)$ and $Y_R = (0.5, 0.4, 0, 8, 10^5, 0, 8, 10^5, 0, 8, 10^5)$.

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