C. R. Acad. Sci. Paris, Ser. I 334 (2002) 927–932

Analyse numérique/*Numerical Analysis*

Closure laws for a two-fluid two-pressure model

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Received 20 February 2002; accepted 15 March 2002

Note presented by Olivier Pironneau.

Abstract Closure laws for interfacial pressure and interfacial velocity are proposed within the frame work of two-pressure two-phase flow models. These enable us to ensure positivity of void fractions, mass fractions and internal energies when investigating field by field waves in the Riemann problem. ***To cite this article: F. Coquel et al., C. R. Acad. Sci. Paris, Ser. I 334 (2002) 927–932.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

Lois de fermeture pour un modèle à deux pressions d’écoulement diphasique

Résumé On propose des lois de fermeture de vitesse et de pression d’interface pour un modèle d’écoulement diphasique à deux pressions. Celles-ci assurent champ par champ de respecter la positivité des fractions volumiques, des variables densité et énergie interne si on examine le problème de Riemann. ***Pour citer cet article : F. Coquel et al., C. R. Acad. Sci. Paris, Ser. I 334 (2002) 927–932.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

Version française abrégée

On examine ici le problème de fermeture apparaissant lorsque l’on souhaite effectuer des simulations d’écoulements diphasiques en retenant l’approche à deux fluides inconditionnellement hyperbolique, ce qui peut être réalisé en privilégiant les formulations basées sur les modèles ne faisant pas l’hypothèse d’équilibre local instantané sous jacente aux modèles « à une pression ». De tels modèles à deux pressions ont été proposés notamment dans [2,9,10,13,6–8,14–16,18]. Ces modèles nécessitent de faire certaines hypothèses concernant le transfert de masse, de quantité de mouvement et d’énergie à l’interface d’une part. La littérature propose pour cela un certain nombre de fermetures locales plus ou moins dédiées. Ils requièrent d’autre part la donnée de la vitesse et de la pression d’interface (qui interviennent explicitement dans l’expression des termes convectifs). On propose donc ici une approche qui permet d’une part de fermer le problème, au sens des relations algébriques, mais également en terme de relation de saut, ce qui est nécessaire puisque le système convectif associé n’admet pas de forme conservative. Une première hypothèse pré-suppose un type topologique de l’interface. Cette hypothèse impose alors trois formes possibles de moyenne pour la vitesse interfaciale. Une seconde hypothèse de fermeture permet d’obtenir une

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S1631-073X(02)02366-X/FLA

inégalité d'entropie physiquement admissible. Elle permet d'obtenir une relation liant vitesse d'interface et pression d'interface. Muni de ces fermetures, on vérifie alors que le problème de Riemann unidimensionnel associé au système convectif non conservatif admet des solutions qui respectent le principe physique de positivité pour les grandeurs fondamentales : densité partielle, fraction volumique et énergie interne. Il est alors en effet possible de fermer le système des relations de saut au voisinage de l'onde associée à la valeur propre $\lambda_1 = V_i$, lorsque l'on a retenu les hypothèses précédentes. Les modèles sont comparés à quelques propositions existantes. Quelques résultats numériques donnent un aperçu du comportement de certains schémas pour un choix de conditions initiales conduisant à une solution instationnaire simple mais d'importance fondamentale. On propose également une voie de modélisation alternative pour le terme de pression interfaciale, qui permet également de fermer le problème aux relations de saut dans tous les champs, dès lors que l'on retient le modèle de vitesse d'interface de base proposé.

1. Introduction

Computation of gas liquid flows requires use of some models. These may rely on the single fluid approach, following for instance the work in [1], or on the two-fluid approach, when one no longer assumes instantaneous local equilibrium of velocity fields (and pressure fields) in each phase. A promising way to deal with this topic consists in using models such as those proposed in [2,9,10,13,15,16,18]. This nonetheless requires specific closures for interfacial velocity and pressure variables, and this is precisely the goal of the present work. In fact it is aimed at providing closures which only require 'obvious' hypothesis on physical background, but also solutions which satisfy positivity requirement for mass fractions, internal energies and volume fractions.

2. Governing equations, closures and main properties

The governing set of equations contains convective terms, source terms and diffusive terms:

$$\big(I + D(W)\big)\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} + C(W)\frac{\partial W}{\partial x} = S(W) + \frac{\partial}{\partial x}\left(E(W)\frac{\partial W}{\partial x}\right) \tag{1}$$

with initial condition $W(x,0) = W_0(x)$, and W, $F(W)$, $G(W)$ and $S(W)$ in $\mathbb{R}^7$, and $C(W)$, $D(W)$, $E(W)$ in $\mathbb{R}^{7\times 7}$. Source terms $S(W)$ account for mass transfer terms, drag effects, energy loss, and other contributions. We set here: $W^t = (\alpha_2, \alpha_2\rho_2, \alpha_2\rho_2 U_2, \alpha_2 E_2, \alpha_1\rho_1, \alpha_1\rho_1 U_1, \alpha_1 E_1)$, where α_2 stands for the void fraction of phase labelled 2, and $\alpha_1 = 1 - \alpha_2$. The density, velocity and total energy within phase k are denoted ρ_k, U_k and E_k respectively. The convective flux is: $F(W)^t = (0, \alpha_2\rho_2 U_2, \alpha_2(\rho_2 U_2^2 + P_2), \alpha_2 U_2(E_2 + P_2), \alpha_1\rho_1 U_1, \alpha_1(\rho_1 U_1^2 + P_1), \alpha_1 U_1(E_1 + P_1))$. Some non-conservative terms are present in governing equations, and viscous terms are accounted for through contribution pertaining to $E(W)$:

$$\begin{cases} D(W)\dfrac{\partial W}{\partial t} = \left(0, 0, 0, P_i\dfrac{\partial \alpha_2}{\partial t}, 0, 0, -P_i\dfrac{\partial \alpha_2}{\partial t}\right), \\ C(W)\dfrac{\partial W}{\partial x} = \left(V_i\dfrac{\partial \alpha_2}{\partial x}, 0, -P_i\dfrac{\partial \alpha_2}{\partial x}, 0, 0, P_i\dfrac{\partial \alpha_2}{\partial x}, 0\right), \\ E(W)\dfrac{\partial W}{\partial x} = \left(0, 0, \alpha_2\mu_2\dfrac{\partial U_2}{\partial x}, \alpha_2\mu_2 U_2\dfrac{\partial U_2}{\partial x}, 0, \alpha_1\mu_1\dfrac{\partial U_1}{\partial x}, \alpha_1\mu_1 U_1\dfrac{\partial U_1}{\partial x}\right). \end{cases} \tag{2}$$

Detailed expression of $S(W)$ may be found in many references. Internal energies e_k are given functions of density ρ_k and pressure P_k within each phase: $e_k = e_k(P_k, \rho_k)$ that obey classical thermodynamic assumptions, and $E_k = 0.5\rho_k U_k U_k + \rho_k e_k$. Assuming that drag terms, mass transfer terms are provided by standard literature, one needs to define both interfacial pressure and velocity fields V_i and P_i. We assume that the interfacial velocity agrees with:

$$V_i(W) = \beta(W)U_1(W) + \big(1 - \beta(W)\big)U_2(W), \quad 0 \leqslant \beta(W) \leqslant 1, \tag{3}$$

for some given function $\beta(W)$. Moreover, we introduce the concept of 'consistancy' property, that is:

$$U_1 = U_2 = U \quad \text{and} \quad P_1 = P_2 = P \quad \text{imply: } P_i = P. \tag{4}$$

The latter enable to account for pressure and velocity non-equilibrium. We recall first that the homogeneous problem associated with the left-hand side of (1) is hyperbolic. It has real eigenvalues $\lambda_1 = V_i$, $\lambda_2 = U_2 - c_2$, $\lambda_3 = U_2$, $\lambda_4 = U_2 + c_2$, $\lambda_5 = U_1 - c_1$, $\lambda_6 = U_1$, $\lambda_7 = U_1 + c_1$, and the right eigenvectors span the whole space $\mathbb{R}^7$ unless $V_i = U_k + c_k$ or $V_i = U_k - c_k$, for $k = 1, 2$. We introduce $m_k = \alpha_k \rho_k$, specific entropies s_k and coefficients a_k, and note:

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

$$\gamma_k P_k \frac{\partial s_k(P_k, \rho_k)}{\partial P_k} + \rho_k \frac{\partial s_k(P_k, \rho_k)}{\partial \rho_k} = 0, \qquad a_k = (s_k)^{-1}\left(\frac{\partial s_k(P_k, \rho_k)}{\partial P_k}\right)\left(\frac{\partial e_k(P_k, \rho_k)}{\partial P_k}\right)^{-1}.$$

Fields associated with the 2-wave, the 4−5-waves and the 7-wave are genuinely nonlinear [11], and the 3-wave and the 6-wave are linearly degenerate.

PROPERTY 1. – The field associated with $\lambda_1 = V_i$ is linearly degenerate if $\beta(W)(1 - \beta(W)) = 0$ or:

$$\beta(W) = (\alpha_1 \rho_1)(\alpha_1 \rho_1 + \alpha_2 \rho_2)^{-1}. \tag{5}$$

Moreover, assuming that $\beta(W) = \beta(\alpha_1, \rho_1, \rho_2, P_1, P_2)$ then the three previous choices are the only ones which ensure that the 1-field is LD.

The proof simply requires us to examine whether: $\nabla_W V_i(W) \cdot r_1(W) = 0$, where $r_1(W)$ stands for the right eigenvector associated with the first eigenvalue. This closure implies that the interface between both phases is infinitely thin, which seems reasonable to obtain a two-fluid model where mixing is expected to be connected with interfacial transfer terms and viscous effects and not to pure convective effects.

When restricting to the third choice (5) for V_i, one may easily compute a family of six independent Riemann invariants through fields associated with λ_p, $p = 2, \ldots, 7$. We only provide here the list of Riemann invariants in the 1-contact discontinuity: $I_1^1(W) = V_i$, $I_2^1(W) = (m_1 + m_2)^{-1} m_1 m_2 (U_1 - U_2)$, $I_3^1(W) = \alpha_1 P_1 + \alpha_2 P_2 + I_2^1(U_1 - U_2)$, $I_5^1(W) = e_1 + \frac{P_1}{\rho_1} + \frac{(I_2^1(W))^2}{2(m_1)^2}$, $I_6^1(W) = e_2 + \frac{P_2}{\rho_2} + \frac{(I_2^1(W))^2}{2(m_2)^2}$. The last one $I_4^1(W)$ cannot be computed unless one provides the explicit form of the interfacial pressure P_i.

2.1. An entropic closure for the interfacial pressure

We now also assume that the following (obviously 'consistant' in the sense of (4)) closure for P_i holds:

$$P_i(W) = \frac{a_1(W)(1 - \beta(W))P_1(W) + a_2(W)\beta(W)P_2(W)}{a_1(W)(1 - \beta(W)) + a_2(W)\beta(W)}. \tag{6}$$

Thanks to this particular choice, the pair (η, F_η) such that: $\eta = -m_1\eta_1 - m_2\eta_2$ where $\eta_k = \mathrm{Log}(s_k) + \psi_k(\alpha_k)$, and $F_\eta = -\mathrm{m}_1\eta_1 U_1 - \mathrm{m}_2\eta_2 U_2$, but also $\psi_1(1 - \alpha_2) = \psi_2(\alpha_2)$, is an entropy–entropy flux pair:

PROPERTY 2. – If $m_k a_k > 0$, closure above ensures that the following entropy inequality holds:

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

One may now compute the last Riemann invariant of the 1-contact discontinuity, that is: $I_4^1 = s_2/s_1$. An advantage of the closure (6) is that this entropy inequality obviously degenerates to give the expected – single phase – entropy inequality on each side of the 1-contact discontinuity. Proposals by Glimm et al. [9]: $P_i = \alpha_2 P_1 + \alpha_1 P_2$, $V_i = \alpha_2 U_1 + \alpha_1 U_2$ are quite different (the 1-wave is GNL). Turning now to the work by Saurel and Abgrall [18], we note that the standard choice of interface velocity belongs to the previous class (5). However, the closure for the interface pressure is completely different from the present one, and takes the form: $P_i = \alpha_1 P_1 + \alpha_2 P_2$. In [13] and [15], closures correspond to $P_i = P_1$ and $V_i = U_2$ (which meets

Properties 1 and 2 with $\beta(W)=0$) where subscript 1 refers to the gas phase. In a recent work [8], authors consider a dual asymmetric formulation, which turns to be: $V_i=U_1$ (in agreement with Property 1) and: $P_i=P_2+\psi(\alpha_2)$. We now focus on the closures (5), (6) and turn to the 'closure' of jump conditions, due to the presence of nonconservative terms. Noting $\hat{\psi}$ some arbitrary average of (ψ_l,ψ_r) and $\Delta\psi=\psi_r-\psi_l$, these may be written:

$$\begin{aligned}
&\left(\widehat{V}_i-\sigma\right)\Delta(\alpha_k)=0,\\
&\Delta\left(m_k(U_k-\sigma)\right)=0,\\
&\Delta\left(m_kU_k(U_k-\sigma)+\alpha_kP_k\right)-\widehat{P}_i\Delta(\alpha_k)=0,\\
&\Delta\left(\alpha_kE_k(U_k-\sigma)+\alpha_kP_kU_k\right)-\widehat{P_iV_i}\Delta(\alpha_k)=0.
\end{aligned}$$

On the left side (or the right side) of the 1-contact discontinuity, these make sense whatever is the definition of $\hat{\phi}$ since $\Delta(\alpha_k)=0$, which results in standard 'single phase' jump relations within each phase, say: $\Delta(\alpha_k)=\Delta(\rho_k(U_k-\sigma))=\Delta(\rho_kU_k(U_k-\sigma)+P_k)=\Delta(E_k(U_k-\sigma)+P_kU_k)=0$. Through the 1-contact discontinuity we get:

$$\begin{aligned}
&\sigma=\widehat{V}_i=(V_i)_l=(V_i)_r,\\
&\Delta\left(m_k(U_k-\sigma)\right)=0\quad\text{for } k=1,2,\\
&\Delta\left(m_1U_1(U_1-\sigma)+\alpha_1P_1\right)+\Delta\left(m_2U_2(U_2-\sigma)+\alpha_2P_2\right)=0,\\
&\Delta\left(\alpha_kE_k(U_k-\sigma)+\alpha_kP_kU_k\right)-\widehat{V}_i\Delta\left(m_kU_k(U_k-\sigma)+\alpha_kP_k\right)=0\quad\text{for } k=1,2.
\end{aligned}$$

One may check that the latter provide the same parametrisation than Riemann invariants I_p^1 listed above. One more jump condition is: $-\sigma\Delta(\eta)+\Delta(F_\eta)=0$, or equivalently $\Delta(\mathrm{Log}(s_2/s_1))=0$. This actually corresponds to the exact connection associated with the last Riemann invariant in the 1-field, that is I_4^1, the form of which has been given above. This last jump condition 'implicitely' provides the counterpart of a 'closure' for the remaining nonconservative product $\widehat{P}_i\Delta(\alpha_k)$.

We will now assume that perfect gas law holds in each phase: $\rho_ke_k=(\gamma_k-1)P_k$. Using previous closures for V_i and P_i, and assuming that $(\alpha_2)_L=(\alpha_2)_R$, the 1D solution of the Riemann problem associated with the above set of equations has a unique entropy consistent solution involving constant states separated by shocks, rarefaction waves and contact discontinuities, provided that some classical condition holds on initial data: $|W_R-W_L|<h(W_L,W_R)$ [11]. Moreover:

PROPERTY 3. – Assume now: $(\alpha_2)_L\neq(\alpha_2)_R$, and also that both $(1-(\alpha_2)_L)(\alpha_2)_L$ and $(1-(\alpha_2)_R)(\alpha_2)_R$ are nonzero. The connection of states through single waves in the 1D solution of the Riemann problem associated with the above set of equations ensures that all states are in agreement with positivity requirements for void fraction, mass fractions and partial pressures assuming perfect gas state law within each phase.

We insist that though the result seems obvious from a physical view point, it is actually not clear whether solutions of the one-dimensional Riemann problem above should agree with the above positivity requirement. Hence the choice of the above closures *a posteriori* ensures that positivity requirements hold.

2.2. An alternative formulation of interfacial pressure

Another 'consistant' way to close the interfacial pressure which seems physically relevant (actually P_i will be constant through the 1-wave) issues from:

$$P_i(W)=F\left(I_1^1(W),I_2^1(W),I_3^1(W),I_4^1(W),I_5^1(W),I_6^1(W)\right)$$

still restricting to the particular choice of interface velocity described above. This actually will provide another physically relevant way to 'close' jump conditions. Recall that since the explicit form of F is now unknown, $I_4^1(W)$ has no explicit form. Nonetheless, we know that $2I_4^1(W) = P_1 - P_2 + (\alpha_1 - \alpha_2)(P_1 + P_2 - 2P_i) + 2I_2^1(W)(U_1 + U_2)$. The objectivity requirement enables to restrict the list of arguments to $I_2^1(W)$, $I_3^1(W)$, $I_5^1(W)$, $I_6^1(W)$. Dimensionless properties imply: $P_i = G(I_3^1(W), I_2^1(W)(I_5^1(W))^{1/2},\ I_2^1(W)(I_6^1(W))^{1/2})$. Owing to 'consistancy' condition (4), one may then require that $G(a,0,0) = a$. Among other choices, an obvious way to close the problem is to choose $G(a,b,c) = a + \mu(\eta|b| + (1-\eta)|c|)$, which obviously agrees with consistancy property, objectivity requirement, but also remains positive provided that μ is positive. The particular choice $G(a,b,c) = a$ corresponds to the closure retained in [19].

3. Numerical results

The overall method relies on the use of the fractional step method strategy, in order to account for source terms first – by providing approximate solutions of $(I + D(W))\partial_t W = S(W)$, and afterwards for convective terms and viscous terms. Computations below have been performed neglecting source terms and viscous terms. We use here an extension (*see* [4]) of original Rusanov scheme and approximate Godunov scheme (introduced in [3]) to the frame of nonconservative systems. The nonconservative variable used for VFRoe-ncv scheme is: $Y^t = (\alpha_2, s_1, U_1, P_1, s_2, U_2, P_2)$. We show here some computational results using CFL $= 0.45$, Figs. 1–9. The number on the x-axis stands for the number of cells. Both results associated with VFRoe-ncv scheme and Rusanov scheme are displayed. Perfect gas EOS have been used within each phase. The counterpart of the test below – in the single phase Euler framework – is the moving contact discontinuity (*see* [1,17,5], …). Despite from its simplicity, it is an important reference since it enables to predict the numerical stability of interfaces. Initial conditions: $(\alpha_1)_L = 0.9$, $(\alpha_2)_L = 0.1$, $(\alpha_1)_R = 0.5$,

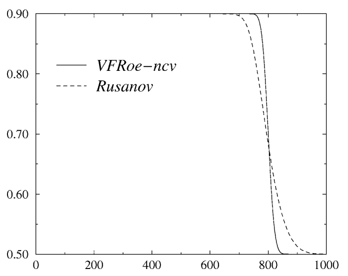

Figure 1. – Void fraction α_1.

Figure 1. – Fraction volumique α_1.

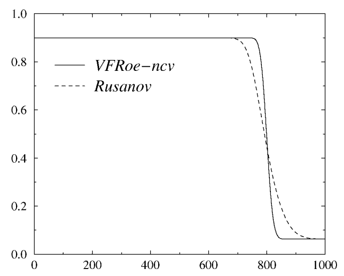

Figure 2. – Partial mass m_1.

Figure 2. – Masse partielle m_1.

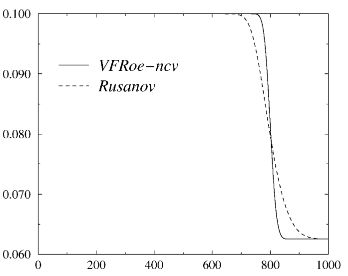

Figure 3. – Partial mass m_2.

Figure 3. – Masse partielle m_2.

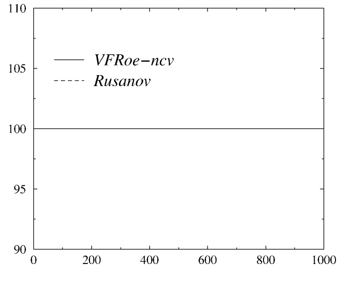

Figure 4. – Interfacial velocity V_i.

Figure 4. – Vitesse d'interface V_i.

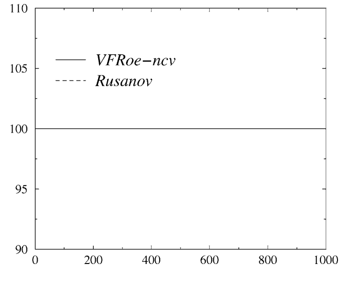

Figure 5. – Velocity U_1.

Figure 5. – Vitesse U_1.

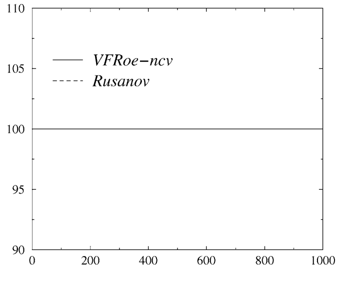

Figure 6. – Velocity U_2.

Figure 6. – Vitesse U_2.

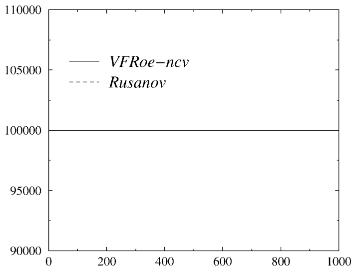

Figure 7. – Interfacial pressure P_i.
Figure 7. – Pression interfaciale P_i.

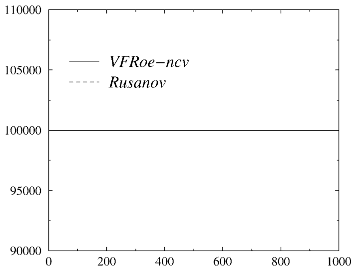

Figure 8. – Pressure P_1.
Figure 8. – Pression P_1.

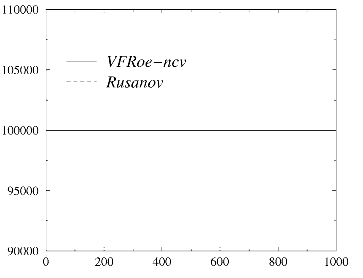

Figure 9. – Pressure P_2.
Figure 9. – Pression P_2.

$(\alpha_2)_R = 0.5$, $(U_1)_L = 100$, $(\tau_1)_L = 1$, $(P_1)_L = 10^5$, $(U_1)_R = 100$, $(\tau_1)_R = 8$, $(P_1)_R = 10^5$, $(U_2)_L = 100$, $(\tau_2)_L = 1$, $(P_2)_L = 10^5$, $(U_2)_R = 100$, $(\tau_2)_R = 8$, $(P_2)_R = 10^5$ are such that a single 1-contact discontinuity is moving to the right. Both velocities and pressures are expected to remain constant.

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