

A FIVE-EQUATION MODEL FOR THE NUMERICAL SIMULATION OF INTERFACES IN TWO-PHASE FLOWS

Titre courant: a five-equation model for two-phase flows

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Abstract. In the Eulerian approach for simulating interfaces in two-phase flows, the main difficulties arise from the fixed character of the mesh which does not follow the interface. Therefore, near the interface there are computational cells containing both fluids which require a suitable modelling of the mixture. Furthermore, most numerical algorithms, such as the volume of fluid or the level set method, involve the transport of a function indicating the localization of each phase. Due to unavoidable numerical diffusion, they have the tendency to thicken this mixture layer around the interface. It is thus necessary to model correctly the two-phase mixture. In the context of compressible gas dynamics we propose such a model, valid for any type of state laws, which satisfies an important property of pressure stability through the interface.

Un modèle à cinq équations pour la simulation numérique des interfaces dans les écoulements diphasiques

Résumé. Dans l'approche eulérienne de la simulation d'interfaces en écoulements diphasiques, les difficultés principales viennent du fait que l'interface ne suit pas le maillage qui reste fixe. Par conséquent, de part et d'autre de l'interface se trouvent des mailles de calcul qui contiennent les deux fluides et pour lesquelles une modélisation appropriée du mélange est requise. De plus, la plupart des algorithmes numériques, comme la méthode du volume de fluide ou des lignes de niveaux, sont basées sur une équation de transport pour une fonction indiquant où se trouve chaque phase. A cause de l'inévitable diffusion numérique, ces méthodes ont tendance à épaissir la couche de mélange autour de l'interface. Il est donc nécessaire de modéliser correctement ce mélange diphasique. Dans le contexte de la dynamique des gaz compressibles nous proposons un tel modèle, valable pour toute loi d'état et qui vérifie une propriété importante de stabilité de la pression à travers l'interface.

Version française abrégée. Dans cette Note nous proposons un modèle de mélange pour deux fluides compressibles, dont les lois d'état sont quelconques, et nous étudions une propriété de stabilité des discontinuités de contact dans ce modèle. La motivation de ce travail est la simulation numérique d'écoulements diphasiques en présence d'interfaces. En effet, lorsqu'on utilise une méthode numérique eulérienne, il y a inévitablement des mailles du domaine de calcul qui contiennent un mélange des deux phases qu'il faut donc savoir modéliser.

Le modèle bifluide, sans terme source, est composé des équations d'Euler pour chacune des phases pures $i = 1, 2$ séparées par une interface

$$\begin{cases} \partial_t \rho_i + \operatorname{div}(\rho_i u_i) = 0 \\ \partial_t(\rho_i u_i) + \operatorname{div}(\rho_i u_i \otimes u_i + p_i I) = 0 \\ \partial_t(\rho_i e_i) + \operatorname{div}((\rho_i e_i + p_i)u_i) = 0 \end{cases} \quad (1)$$

où $\rho_i, u_i, p_i, \epsilon_i, e_i$ sont respectivement la densité, la vitesse, la pression, l'énergie interne et l'énergie interne spécifique totale définie par $e_i = \epsilon_i + |u_i|^2/2$. L'équation d'état (EOS) est $p_i = p_i(\rho_i, \epsilon_i)$.

Le système (1) est accompagné de conditions de saut à l'interface de normale unité orientée n et de vitesse normale σ

$$[\rho]\sigma = [\rho u] \cdot n, \quad [\rho u]\sigma = [\rho u \otimes u + pI]n, \quad [\rho e]\sigma = [(\rho e + p)u] \cdot n, \quad (2)$$

avec $[f] = f_1 - f_2$ le saut d'une quantité f à travers l'interface. A l'aide des variables de mélange (3), on peut réécrire (1-2) comme un système global (4-5) de quatre équations: les trois équations (4) de conservation de la masse, de la quantité de mouvement et de l'énergie, auxquelles on ajoute une équation (5) de transport de la fraction volumique.

Lorsque les deux fluides sont des gaz parfaits, un modèle très simple, dit à quatre équations, a été étudié par Abgrall [1] et Karni [6]. Il consiste à fermer le système (4-5) en supposant les températures et pressions des deux fluides égales. D'un point de vue numérique, ce système écrit sous forme conservative a le défaut d'engendrer des oscillations numériques (mais non physiques) de la pression à travers une interface. Pour remédier à cet inconvénient, il est essentiel d'écrire l'équation de transport (5) sous une forme non conservative convenable (voir [1], [6]). Cette approche a été généralisée à d'autres types de lois d'état, comme les gaz raides ou les gaz de van der Waals (voir [13], [14], [16]). Tous ces travaux utilisent encore une forme algébrique particulière des lois d'état.

Pour pouvoir traiter des lois d'état quelconques (ce qui est courant dans les applications pratiques), nous proposons un nouveau modèle à cinq équations qui s'obtient en ajoutant aux quatre équations du modèle précédent une équation de conservation d'une des deux masses phasiques. On obtient ainsi le système (7) qui ne nécessite plus qu'une seule relation de fermeture algébrique. Parmi diverses possibilités analysées dans [2], nous sélectionnons l'hypothèse d'isobarie du mélange (égalité des pressions) qui permet d'obtenir un résultat de stabilité numérique à l'interface entre les deux phases.

Nous montrons tout d'abord que ce système à cinq équations avec fermeture isobarique est bien posé au sens suivant. A partir des quantités conservées on peut calculer toutes les variables thermodynamiques de chaque phase, et en particulier la pression commune. De plus le système est hyperbolique avec une expression explicite des valeurs et vecteurs propres de la jacobienne.

Le résultat principal de stabilité s'énonce comme suit (voir la Proposition 5.1). On considère une discontinuité de contact vérifiant (9) (c'est-à-dire que seule la fraction volumique est discontinue). On utilise une méthode numérique de type Godunov basée sur un solveur approché de Riemann qui préserve exactement les discontinuités de contact (par exemple, le schéma de Roe, celui d'Osher ou AUSM). Alors, la solution numérique est encore une discontinuité de contact (malgré l'étape de moyennisation sur chaque maille à la fin d'un pas de temps), et en particulier la vitesse et la pression restent uniformes à travers l'interface. Ce résultat justifie l'utilisation pratique de notre modèle à cinq équations.

1 Introduction

We consider the motion of two compressible fluids separated by a sharp interface. For simplicity we assume both fluids are immiscible, *i.e.* there is no phase change and mass transfert at the interface, and we neglect all source terms and diffusive terms (see [7] for a generalization). The resulting system of first order hyperbolic conservation laws is (1) for each phase $i = 1, 2$, separated by an interface where the jump conditions (2) hold true. System (1-2) can be rewritten as a global model for the bulk fluid made by the juxtaposition of its two phases. Introducing a "color function" $z(x)$ which is the characteristic function of phase 1 ($z(x) = 1$ in phase 1 and $z(x) = 0$ in phase 2), we define global variables

$$\rho = z\rho_1 + (1 - z)\rho_2, \quad \rho e = z\rho_1 e_1 + (1 - z)\rho_2 e_2, \quad p = zp_1 + (1 - z)p_2, \quad u = zu_1 + (1 - z)u_2, \quad (3)$$

which satisfy

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho u) = 0 \\ \partial_t(\rho u) + \operatorname{div}(\rho u \otimes u + pI) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + p)u) = 0 \end{cases} \quad (4)$$

together with the advection of the color function

$$\partial_t z + u \cdot \nabla z = 0. \quad (5)$$

System (4-5), in its weak form or variational formulation, includes the jump conditions at the interface. Of course, both systems (1-2) and (4-5) are provided with an entropy condition that we do not specify.

From a numerical point of view, Lagrangian methods such as front-tracking can solve very accurately system (1-2) since the mesh follows adaptively the interface, but they are very costly and difficult to implement in three dimensions. Eulerian methods, being much cheaper, are more popular (*e.g.* the volume of fluid method [5], [8], the level set method [10], [11], [15], or the ghost fluid method [3]). They capture the interface, rather than track it on a fixed mesh. However, their main drawback, as for any front-capturing method, is that they smear out the interface. In other words, instead of computing a sharp interface, we obtain a small layer of cells around the true interface in which we have a mixture of both fluids. Although this transition layer has no special physical meaning and is a purely numerical artefact, we have to model it in order to globally compute the hydrodynamics of the two phases in the whole domain. It is not difficult to define global averaged conservative variables, but the main point is to compute the resulting pressure in a two-phase zone, *i.e.* to define a suitable “mixture law” or generalized EOS that will nicely degenerate to the pure phase EOS in the pure fluid areas. In the case of perfect gases Abgrall [1] (see also [6]) gave such a mixture law which corresponds to the well-known Dalton law for mixture of different species. Saurel and Abgrall [13], [14] extended this approach to so-called stiffened gas, while Shyue [16] treated the case of van der Waals or Mie-Grüneisen type gas. In all cases a common numerical difficulty is the occurrence of pressure oscillations through material interfaces. As a remedy to this problem the previous authors provide various fixes of the numerical schemes used for solving (4-5). Here, we generalize these previous works to the case of real gas with arbitrary EOS. The main idea is to use a new five-equation model for the mixture, *i.e.* we add one more equation to system (4-5) which is a phase mass balance. Furthermore, this model enjoys a stability property for the pressure at material interfaces which implies that no numerical fix is required for a large class of numerical scheme based on approximate Riemann solvers.

2 Mixture law for perfect gas

The purpose of this section is to describe a very simple and classical model used for the isothermal mixing of perfect gases (see *e.g.* [1]). We recall this four-equation model just for the sake of comparison. We keep the notations of the introduction and the four equations of the model are still (4-5), but now $z(x)$ becomes the volume fraction of fluid 1 at point x , which takes its values in the range $[0, 1]$. For simplicity we shall often use the notation $z_1 = z$ and $z_2 = 1 - z$. In the sequel we assume that, in the mixture, the two fluids have the same velocity, *i.e.* $u_1 = u_2 = u$. This implies that we can define a mixture internal energy ϵ which satisfies

$$\rho \epsilon = z_1 \rho_1 \epsilon_1 + z_2 \rho_2 \epsilon_2, \quad e = \epsilon + |u|^2/2. \quad (6)$$

Let us denote by c_{vi} , c_{pi} , respectively the specific heat at constant volume and pressure of the i^{th} fluid. If we denote by T_i its temperature, we have $\epsilon_i = c_{vi} T_i$, $p_i = (\gamma_i - 1) \rho_i \epsilon_i$, and $\gamma_i = c_{pi} / c_{vi}$. During the computation, there will be cells containing both fluids near the interface, and a new

EOS for this mixture is required if one want to treat it as a single equivalent fluid. The four-equation model is closed thanks to two physical assumptions. First, the two species are assumed to be in thermal equilibrium in the mixture, *i.e.* they share the same temperature T . Second, Dalton's law applies which, in our notations, means pressure equilibrium, *i.e.* $p_1 = p_2 = p$. Introducing thermodynamic parameters for the mixture

$$\rho c_p = z_1 \rho_1 c_{p1} + z_2 \rho_2 c_{p2}, \quad \rho c_v = z_1 \rho_1 c_{v1} + z_2 \rho_2 c_{v2}, \quad \gamma = c_p / c_v,$$

the mixture EOS is found to be $\epsilon = c_v T$, and $p = (\gamma - 1) \rho \epsilon$. It is similar to that of a perfect gas, except that the γ parameter depends on the mass fractions. One can also check that the volume average of the entropies is indeed an entropy for the mixture. This mixing process has been generalized to wider classes of gas, *e.g.* stiffened gas [13] or van der Waals gas [16]. There are also other possible mixing laws which allow to define an EOS for the mixture: in [9] the isothermal assumption is replaced by the assumption $T_1 ds_1 = T_2 ds_2$ where s_i is the entropy of fluid i . In any case, the purpose of this type of modelization is to view the mixture zone (as well as the entire domain) as occupied by a single equivalent fluid.

3 The five-equation model

We still assume that in the mixture both fluids have the same velocity u , and that the average mixture variables are defined by (3) and (6). Our five-equation model is obtained by adding to the four previous equations (4-5) a phase mass conservation. It is thus equivalent to

$$\left\{ \begin{array}{l} \partial_t(z_1 \rho_1) + \operatorname{div}(z_1 \rho_1 u) = 0 \\ \partial_t(z_2 \rho_2) + \operatorname{div}(z_2 \rho_2 u) = 0 \\ \partial_t(\rho u) + \operatorname{div}(\rho u \otimes u + pI) = 0 \\ \partial_t(\rho e) + \operatorname{div}((\rho e + p)u) = 0 \\ \partial_t z + u \cdot \nabla z = 0. \end{array} \right. \quad (7)$$

Remark that, if initially at time $t = 0$ we have $z \in \{0, 1\}$, then at later times the exact solution will still satisfy $z \in \{0, 1\}$, and system (7) is equivalent to the original system (4-5). Of course, the interest of (7) is that it can handle mixture zones where $z \in]0, 1[$. This system of five equations (in 1-D, or seven equations in 3-D) describes the motion of the two fluids in terms of the following six variables (in 1-D, or eight variables in 3-D): $z, \rho_1, \rho_2, u, \epsilon_1, \epsilon_2$. The above system is thus not closed and we need another algebraic relation to close it. One way of understanding this missing closure relation is to see that it is not possible to compute the pressure p with the sole knowledge of the conserved quantities in (7). Indeed, these conserved quantities yield the values of z, ρ_1, ρ_2, u but not that of ϵ_1, ϵ_2 (merely a linear combination of them is known). Therefore, this extra constitutive hypothesis can be thought of as a definition of a "generalized EOS" for the mixture. Of course, there are many possible closure relations that allows to recover the pressure p , but among them we select those that allows to recover all the thermodynamic variables of each fluid (it is easy to see that not all of them have this property). We call this selection principle a consistency property since it is physically, as well as numerically, sound to be able to characterize completely each fluid in a mixture model as above.

We suggest three different consistent closure laws based on reasonable physical assumptions that we analyse from a mathematical and numerical point of view: the isobaric closure, the isothermal closure, and the iso-heat-deposition closure. For each of them we study in [2] the consistency and the hyperbolicity of the system, as well as some qualitative properties of interface advection. Here we focus on the isobaric closure which is the most interesting one from a numerical point of view.

4 Isobaric closure

To close system (7) we assume equality of the phase pressures, *i.e.* $p_1 = p_2$. Denoting by $p_i(\rho_i, \rho_i \epsilon_i)$ the EOS of fluid i , we introduce the derivatives $\delta_i = \partial(\rho_i \epsilon_i)/\partial \rho_i$ and $\xi_i = \partial(\rho_i \epsilon_i)/\partial p_i$. Denoting by h_i the specific enthalpy, defined as $\rho_i h_i = \rho_i \epsilon_i + p_i$, the speed of sound is $c_i^2 = (h_i - \delta_i)/\xi_i$. We first show that under a mild assumption on each phase EOS, all phase variables $z, \rho_1, \rho_2, u, \epsilon_1, \epsilon_2$ can be recovered from the knowledge of the global conserved quantities $z_1 \rho_1, z_2 \rho_2, \rho u, \rho e, z$. It is enough to check that one can compute the pressure from the conserved variables.

Proposition 4.1. *Under the hypothesis $\xi_i > 0$ on each phase EOS, the isobaric closure $p_1 = p_2 = p$ allows to define the pressure p as a single-valued function of $z, \rho_1, \rho_2, \rho e$.*

Proof. We need to prove that for given values $\rho e, \rho_1, \rho_2 > 0$ and $z \in [0, 1]$ the algebraic system

$$p_1(\rho_1, \rho_1 \epsilon_1) = p_2(\rho_2, \rho_2 \epsilon_2), \quad z \rho_1 \epsilon_1 + (1 - z) \rho_2 \epsilon_2 = \rho e,$$

has always one and only one solution $(\rho_1 \epsilon_1, \rho_2 \epsilon_2)$. Introducing $x = (\rho_1 \epsilon_1)/(\rho e)$ this is equivalent to show that

$$\phi(x) = p_1(\rho_1, \rho e x) - p_2\left(\rho_2, \frac{1 - zx}{1 - z} \rho e\right)$$

has a single zero in $[0, 1]$. Thanks to the hypothesis $\xi_i > 0$, its derivative is easily shown to be positive on $[0, 1]$. Since $\phi(1) = p_1(\rho_1, \rho e) \geq 0$ and $\phi(0) = -p_2(\rho_2, \rho e) \leq 0$, there exists a unique $x_0 \in [0, 1]$ such that $\phi(x_0) = 0$. \square

To show that system (7) is well-posed, *i.e.* is hyperbolic, we rewrite it in terms of the following primitive variables $W = (z \rho_1, (1 - z) \rho_2, u, p, z)$. After some calculation, in 1-D we obtain

$$\frac{\partial W}{\partial t} + \begin{pmatrix} u & 0 & z \rho_1 & 0 & 0 \\ 0 & u & (1 - z) \rho_2 & 0 & 0 \\ 0 & 0 & u & \frac{1}{\rho} & 0 \\ 0 & 0 & \rho c^2 & u & 0 \\ 0 & 0 & 0 & 0 & u \end{pmatrix} \frac{\partial W}{\partial x} = 0. \quad (8)$$

with the mixture speed of sound c defined by $\rho c^2 = (z_1 \rho_1 \xi_1 c_1^2 + z_2 \rho_2 \xi_2 c_2^2)/(z_1 \xi_1 + z_2 \xi_2)$. Then, it is easy to diagonalize this Jacobian matrix.

Proposition 4.2. *The five-equation system (7) with isobaric closure is hyperbolic. The eigenvalues of the Jacobian matrix are $\lambda_1 = u - c$, $\lambda_2 = \lambda_3 = \lambda_4 = u$, and $\lambda_5 = u + c$. The corresponding right eigenvectors are*

$$\begin{aligned} r_1 &= (z \rho_1, (1 - z) \rho_2, c, \rho c^2, 0) \\ r_2 &= (1, 0, 0, 0, 0) \\ r_3 &= (0, 1, 0, 0, 0) \\ r_4 &= (0, 0, 0, 0, 1) \\ r_5 &= (-z \rho_1, -(1 - z) \rho_2, -c, \rho c^2, 0) \end{aligned}$$

5 Pressure stability through a material interface

We now show that the above five-equation model enjoys a stability property for the pressure at material interfaces for a large class of numerical scheme based on approximate Riemann solvers, including Roe, Osher, and AUSM scheme (see *e.g.* [4], [17]). To simplify, we work in one space dimension. We consider a material interface, *i.e.* a discontinuity separating constant right and left states (indexed by R and L) satisfying

$$u^L = u^R = u, \quad p^L = p^R = p, \quad \rho_i^L = \rho_i^R = \rho_i, \quad \text{for } i = 1, 2. \quad (9)$$

By using the EOS, this implies that the phase internal energies are equal through the interface, *i.e.* $\epsilon_i^L = \epsilon_i^R$, but of course, since the color function z is discontinuous, the mixture density and energy is also discontinuous, *i.e.* $\rho_L \neq \rho_R$, $\epsilon_L \neq \epsilon_R$. Clearly, the exact solution of this Riemann problem is a contact discontinuity propagating at velocity u and separating the above constant right and left states. Numerically we solve this problem by Godunov method based on an approximate Riemann solver which preserves exactly such contact discontinuities. There are many solvers with such a property, including Roe, Osher, and AUSM schemes.

Proposition 5.1. *The discrete solution of the Riemann problem with data satisfying (9), obtained with such a numerical method, has constant pressure p , velocity u , and phase densities ρ_i for all times.*

Proof. Let $\sigma = u\delta t/\delta x$ be the Courant number. The downstream state (indexed by $*$) after a time step δt , and after cell averaging, is given by

$$\begin{aligned} z^* &= \sigma z^L + (1 - \sigma)z^R, \\ \rho_i^* z_i^* &= \sigma \rho_i^L z_i^L + (1 - \sigma)\rho_i^R z_i^R, \\ \rho^* u^* &= \sigma \rho^L u^L + (1 - \sigma)\rho^R u^R, \\ \rho^*(\epsilon^* + (u^*)^2/2) &= \sigma \rho^L(\epsilon^L + (u^L)^2/2) + (1 - \sigma)\rho^R(\epsilon^R + (u^R)^2/2). \end{aligned} \quad (10)$$

Combining (9) and the definition $\rho^* = z_1^* \rho_1^* + z_2^* \rho_2^*$, the three first lines of (10) yield $\rho_i^* = \rho_i$ and $u^* = u$. The last line of (10) gives

$$\rho^* \epsilon^* = \sigma \rho^L \epsilon^L + (1 - \sigma)\rho^R \epsilon^R = \sum_{i=1,2} (\sigma z_i^L + (1 - \sigma)z_i^R) \rho_i \epsilon_i = \sum_{i=1,2} z_i^* \rho_i \epsilon_i. \quad (11)$$

By Proposition 4.1, equation (11) together with $p_1(\rho_1^*, \rho_1 \epsilon_1) = p_2(\rho_2^*, \rho_2 \epsilon_2)$ has a unique solution $(\rho_1 \epsilon_1, \rho_2 \epsilon_2)$. Since $p_1^*(\rho_1^*, \rho_1^* \epsilon_1^*) = p_2^*(\rho_2^*, \rho_2^* \epsilon_2^*)$ and $\rho^* \epsilon^* = \sum_{i=1,2} z_i^* \rho_i^* \epsilon_i^*$, by uniqueness we have $\rho_i^* \epsilon_i^* = \rho_i \epsilon_i$. Finally, $\rho_i^* = \rho_i$ implies that $\epsilon_i^* = \epsilon_i$ and thus $p^* = p$. \square

6 Conclusion

The five-equation model with isobaric closure is a hyperbolic model suitable for two-phase flows with interfaces. Although the model is not written in conservation form, the mass of both fluids is conserved as well as the total momentum and energy. Unlike other models, it allows a correct simulation of interface motion with a standard conservative Godunov-type scheme (at first and second order). Numerical experiments are consistent with this analysis (see [2]). In the case of two perfect gases, our model is equivalent to that of Shyue [16]. However, it can be used for arbitrary equations of state.

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