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le 16 octobre 2006

**Couplage interfacial instationnaire
de modèles diphasiques**

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Chapitre 1

Introduction

De nombreux codes industriels ont été développés par EDF-R&D (Electricité de France - Recherche et Développement) et le CEA (Commissariat à l’Energie Atomique) pour simuler le comportement des fluides dans les circuits hydrauliques des centrales nucléaires à eau pressurisée. L’effort commun d’EDF et du CEA, appuyé par l’IRSN (Institut de Radioprotection et de Sûreté Nucléaire) et FRAMATOME-ANP, pour créer une synergie dans ce domaine a abouti, en 2001, à la création du projet de codéveloppement NEPTUNE. L’objectif de ce projet est de construire la prochaine génération de codes de calcul simulant les écoulements diphasiques eau-vapeur dans le domaine nucléaire. La plateforme¹ permettra une simulation multi-échelles en temps réel. Il y a quatre échelles de modélisation des phénomènes physiques, de la plus grossière à la plus fine, celles-ci sont :

- l’échelle système, où la centrale est représentée dans sa globalité et dont l’échelle caractéristique est le mètre ;
- l’échelle composant, dont l’échelle caractéristique est le centimètre ;
- l’échelle mésoscopique, pour laquelle on prend en compte les phénomènes de l’ordre du millimètre.
- l’échelle microscopique, qui correspond à la simulation numérique directe (DNS).

L’utilisation de ces différentes échelles de simulation permettra d’améliorer la prédiction des comportements d’une centrale nucléaire, avec comme objectifs d’accroître le niveau de sûreté et d’obtenir une meilleure compétitivité économique.

Les différents travaux composant le projet NEPTUNE ont été regroupés selon trois axes complémentaires :

- le développement logiciel ;
- une action de recherche physique et numérique ;
- l’expérimentation physique et le développement de techniques de mesures pour les fluides diphasiques.

Ce travail de thèse s’inscrit dans l’action de recherche numérique. Il a pour but de proposer des méthodes mathématiques et numériques permettant de réaliser le *couplage des différents codes* de thermo-hydraulique basés sur la *technique des Volumes Finis*. Ce couplage sera *interfacial*, cela veut dire que les codes à coupler ne devront en aucun cas être modifiés. Ce transfert d’information entre codes se fera en prescrivant des conditions aux limites sous forme de flux.

1. La plate-forme logicielle résultat de cet effort commun couvrira l’ensemble des échelles de simulation et permettra la mise en oeuvre de couplages multi-échelles

Afin de mieux appréhender la diversité des codes utilisés (et donc les différentes échelles de modélisation) dans le domaine de la thermo-hydraulique nucléaire, une courte description d'une centrale nucléaire avec un Réacteur à Eau Pressurisée (ou REP) est utile. Un schéma simplifié de centrale REP est donné par la figure (1.1). Ce type de centrale est composé de trois circuits hydrauliques "indépendants" : le circuit primaire, le circuit secondaire et le circuit de refroidissement. Le circuit primaire est un circuit fermé dont l'eau est à une pression avoisinant les 155 bar, avec une densité voisine de 700 kg/m^3 et une température entre $290 \text{ }^\circ\text{C}$ et $325 \text{ }^\circ\text{C}$. Sauf accident, ce circuit contient principalement de l'eau et très peu de vapeur. La pompe du circuit primaire envoie l'eau dans la cuve où elle se réchauffe en passant à travers les assemblages de combustible du coeur. Cette eau rejoint ensuite le générateur de vapeur qui est un échangeur thermique avec le circuit secondaire. Dans celui-ci de l'eau "froide", ayant une température de l'ordre de $230 \text{ }^\circ\text{C}$, est propulsée par la pompe dans le générateur de vapeur. Au contact des tubes dans lesquels circule l'eau du primaire elle se transforme en vapeur à $290 \text{ }^\circ\text{C}$ pour une pression de 75 bar. C'est cette vapeur qui sert à entraîner la turbine génératrice de courant. En sortie de turbine, la vapeur pénètre dans le condenseur où elle est retransformée en eau. Le dernier circuit est le circuit de refroidissement, c'est le seul circuit à être ouvert, on y retrouve des conditions de température et pression "normales" (pression de 1 bar et température de $10 \text{ }^\circ\text{C}$ à $30 \text{ }^\circ\text{C}$). De l'eau froide, provenant d'une rivière ou de la mer, est injectée dans le condenseur et permet de condenser la vapeur du secondaire ; elle est ensuite refroidie grâce à l'aéroréfrigérant qui permet de dégager une partie de la chaleur dans l'atmosphère, puis retourne dans l'environnement.

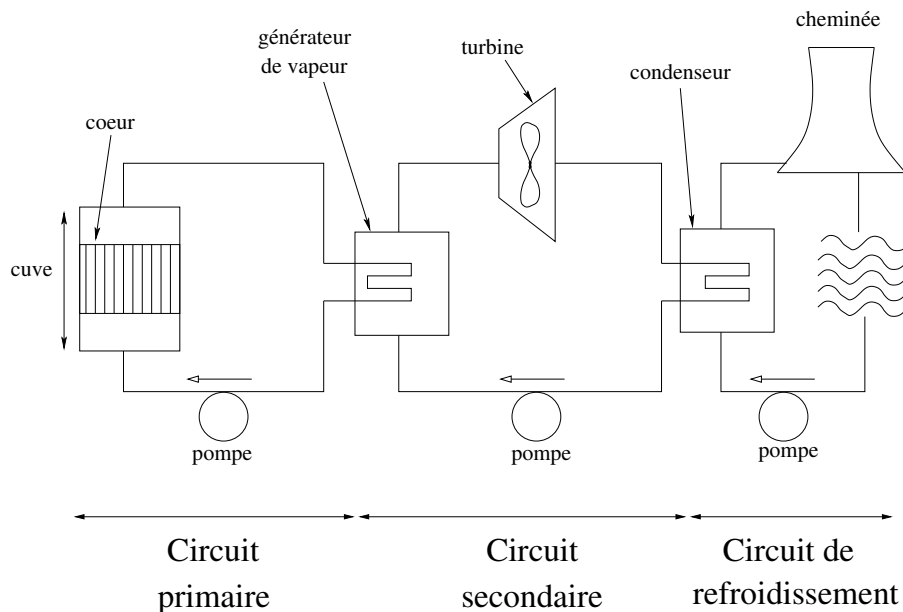


FIG. 1.1 – Schéma des principaux organes des circuits hydrauliques d'une centrale nucléaire avec un coeur à eau pressurisée. Le sens des flèches indique le sens de circulation du fluide en régime non-accidentel.

Nous allons maintenant nous concentrer sur le circuit primaire. Différents modèles de thermo-hydraulique sont utilisés dans les différentes parties de ce circuit. Le coût en temps de calcul d'un code de simulation d'écoulement thermo-hydraulique est fonction de trois paramètres : le nombre de mailles permettant de discrétiser le domaine de calcul, la finesse de représentation des phénomènes

physiques, et les schémas numériques utilisés pour discrétiser le système d'équations. Le deuxième paramètre est directement lié au nombre d'équations, et donc de variables, entrant dans la composition du modèle. Dans certains domaines de calcul nécessitant un nombre de mailles restreint on peut donc se permettre d'augmenter la finesse de représentation du modèle; et inversement, si l'on veut une grande finesse de modélisation on devra se contenter d'un nombre réduit de mailles pour conserver un temps de calcul raisonnable (le temps réel est un objectif important). Le tableau et la figure ci-dessous présente une configuration possible pour l'utilisation des différents codes de calcul.

	3D poreux	3D libre	1D poreux	1D libre	0D
NEPTUNE_CFD		X			
FLICA IV	X				
THYC	X				
CATHARE			X	X	X
GENEPI	X				

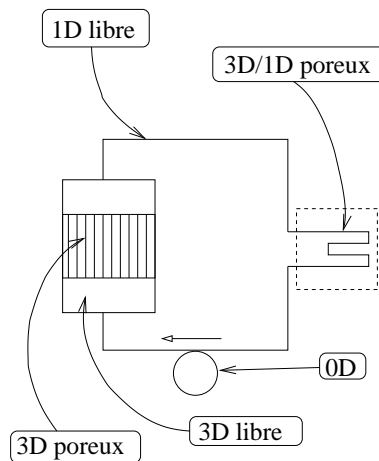


FIG. 1.2 – Circuit primaire et un choix de modélisation associé

Parmi les codes cités dans le tableau ci-dessus le code GENEPI, utilisé pour les simulations de générateurs de vapeur, est basé sur la technique des Eléments Finis; il sort du cadre de notre étude. Les autres codes de calcul ont comme point commun d'utiliser des méthodes basées sur la technique des Volumes Finis. Voilà une courte description de chacun d'eux :

- NEPTUNE_CFD : *modèle* bi-fluide standard à une pression, six équations (2 équations de masse, 2 équations de quantité de mouvement, 2 équations d'énergie totale), *schéma numérique* du type prédicteur/correcteur en pression sur maillage colocalisé.
- FLICA IV : *modèle* homogénéisé à 4 équations (2 équations de masse, 1 équation de quantité de mouvement, 1 équation d'énergie totale), *schéma numérique* de type hyperbolique (schéma de Roe) sur maillage colocalisé.
- THYC : *modèle* homogénéisé 3 ou 4 équations (1 ou 2 équation(s) de masse, 1 équation de quantité de mouvement, 1 équation d'énergie totale), *schéma numérique* du type prédicteur/correcteur en pression sur maillage décalé.
- CATHARE : *modèle* bi-fluide standard à une pression, six équations (2 équations de masse, 2 équations de quantité de mouvement, 2 équations d'énergie totale), *schéma numérique* du

type prédicteur/correcteur en pression sur maillage décalé.

Le code CATHARE permet de simuler le circuit primaire dans son ensemble en utilisant à peu près un millier de mailles. Cette représentation à l'échelle système du circuit primaire permet une simulation en temps réel mais reste peu précise, eu égard à l'échelle des mailles utilisées.

Les schémas numériques associés aux codes de calcul ci-dessus ont un principe commun. Les variables discrétisées sont uniformes sur chaque maille du domaine discret et la mise à jour des grandeurs d'une cellule est réalisée en effectuant un bilan des flux traversant les faces de cette cellule. Dans les faits la différence entre les schémas numériques utilisés réside dans la manière d'estimer ces flux. Ainsi le couplage de deux codes de calcul différents ayant une frontière commune se fera par prescription des flux aux faces des cellules jointes. Cette frontière, constituée d'une ou plusieurs faces sera appelée dans la suite interface de couplage. La difficulté du couplage de codes de calcul différents réside donc dans la définition des flux aux interfaces de couplage, ceux-ci servant de conditions aux limites pour chacun des codes. Ces flux de couplage doivent notamment prendre en compte les éventuelles incompatibilités entre les modèles mis en présence de part et d'autre des interfaces de couplage.

Afin de clarifier la suite de l'exposé nous considérerons le cas du couplage de deux modèles de part et d'autre d'une interface de couplage composée d'une unique face que nous supposons verticale; nous distinguerons les modèles (resp. flux, systèmes d'équations, états, ...) droit et gauche comme étant les modèles (resp. flux, systèmes d'équations, états, ...) à droite et à gauche de cette interface de couplage. On suppose donc ici que les maillages sont colocalisés, c'est-à-dire que deux cellules voisines n'ont qu'une unique face en commun. Il est prévu, dans le cadre du projet NEPTUNE, d'étendre les travaux présentés dans cette thèse aux maillages non-colocalisés appelés aussi maillages décalés. Actuellement deux approches sont possibles afin de calculer les flux de couplages et bien qu'elles puissent coïncider, elles restent basées sur des idées différentes. La première approche est issue du formalisme proposé par A.Y. Leroux [44] pour le traitement des termes sources. Un "modèle père" est introduit au niveau de l'interface de couplage. Celui-ci dégénère vers le modèle droit et vers le modèle gauche; cette propriété de filiation permet d'assurer *en partie* la cohérence du couplage. En outre, ce modèle permet le calcul des flux de couplage par la résolution d'un unique problème de Riemann dont les données initiales sont issues des états gauche et droit. C'est principalement sur des méthodes dérivées de cette approche que porteront nos efforts par la suite. La deuxième approche a été proposée par E. Godlewski et P.A. Raviart [39],[38]. Cette méthode nécessite la résolution de deux problèmes de Riemann au niveau de l'interface. Le flux de couplage pour le modèle droit (resp. gauche) est calculé à partir du problème de Riemann associant le système d'équations droit (resp. gauche) et les états droit et gauche. Il est à noter que le choix des informations issues des états droit et gauche (à l'aide de changements de variables) a une influence sur les résultats du couplage. Cela permet donc, dans une certaine mesure, de choisir les propriétés associées au couplage. Cette approche est largement utilisée par le groupe de travail sur le couplage interfacial de modèles [5] commun au laboratoire Jacques Louis Lions et au laboratoire SFME du CEA. Par ailleurs, certains groupes de travail ont choisi des orientations radicalement différentes pour coupler des modèles différents. Le "Center for Integrated Turbulence Simulations" de l'université de Stanford (voir <http://www.stanford.edu/group/cits/>) ou l'unité "Community Climate System Model" (voir <http://www.cesm.ucar.edu/models/ccsm3.0/cpl6/>) proposent des méthodes principalement basées sur la reconstruction de données par interpolation.

Pour mieux appréhender les problèmes de compatibilité d'information, plusieurs problèmes "élémentaires" vont être successivement abordés. Le premier problème, abordé dans le chapitre 2, est un problème préliminaire au couplage proprement dit, il s'agit de choisir une méthode permettant le traitement des termes sources dans le cadre de régimes instationnaires. Ce travail était initialement motivé par l'approche de couplage visée à terme. Les stratégies de couplage retenues dans les chapitres 4 et 5 font appel structurellement aux techniques d'éclatement d'opérateur ; l'alternative examinée sur la plan numérique dans le chapitre 2 n'est pas retenue. Une approche est ensuite proposée au chapitre 3 afin de coupler un code "travaillant" sur des domaines mono-dimensionnels et un code "travaillant" sur des domaines tridimensionnels et tous deux basés sur les équations d'Euler isentropique. Dans le quatrième chapitre nous abordons le problème du couplage de deux modèles d'écoulement diphasique homogénéisé, un modèle relaxé (Homogeneous Relaxed Model) et un modèle équilibré (Homogeneous Equilibrium Model). Le cinquième chapitre présente un cas de couplage pseudo-industriel réalisé grâce aux méthodes étudiées dans les premiers chapitres. Deux annexes principales complètent ce document. La première propose une méthode utilisant un modèle bi-fluide à deux pressions relaxé pour simuler un modèle bi-fluide standard à une pression. La deuxième annexe est une extension du travail du chapitre 3, il s'agit d'appliquer les méthodes proposées dans le cadre des équations isentropiques d'Euler au cadre des systèmes d'équations basés sur le système d'Euler.

Chapitre 2 : Étude comparative de schémas numériques pour les systèmes hyperboliques avec termes sources en régime instationnaire

Les modèles sur lesquels sont basés les codes de calcul présentés ci-dessus possèdent tous des termes sources. Les systèmes d'équations non-homogènes, que nous supposons conservatives, s'écrivent alors :

$$\partial_t (W) + \partial_x (F(W)) = S(W) \quad (1.1)$$

Ce premier chapitre présente trois schémas numériques basés sur deux techniques différentes permettant le traitement numérique des termes sources $S(W)$ d'ordre zéro.

La première approche repose sur la technique classique de pas fractionnaires [80], celle-ci sépare l'opérateur de convection (1.2) et l'opérateur associé aux termes sources (1.3). Le schéma numérique permettant de calculer l'approximation de la solution au temps $t^{n+1} = t^n + \Delta t$ à partir de l'approximation de la solution au temps t^n s'écrit alors :

$$\partial_t (W^1) + \partial_x (F(W^1)) = 0, \quad \text{avec } W^1(x, t = 0) = W(x, t^n) \quad (1.2)$$

$$\partial_t (W^2) = S(W^2), \quad \text{avec } W^2(x, t = 0) = W^1(x, t = \Delta t) \quad (1.3)$$

La solution approchée au temps t^{n+1} est alors $W(x, t^{n+1}) = W^2(x, \Delta t)$. La deuxième technique est issue des travaux [44] visant à obtenir de bonnes approximations des équilibres stationnaires entre termes sources et termes de convection sur maillage grossier. Dans le cas de solutions en régime stationnaire, les méthodes de type pas fractionnaires peuvent en effet manquer de précision sur maillage grossier. L'idée est donc de traiter de manière synchrone les effets de convection et les termes sources. Pour ce faire on "décentre" les termes sources pour les inclure dans le calcul des flux à travers les interfaces ; on introduit une variable $A(x, t)$ définie partiellement par ses dérivées

partielles : $\partial_t (A) = 0$ et $\partial_x (A) = 1$. Le calcul des flux aux interfaces est alors réalisé en considérant le système homogène non-conservatif :

$$\partial_t (A) = 0 \tag{1.4}$$

$$\partial_t (W) + \partial_x (F(W)) - S(W)\partial_x (A) = 0 \tag{1.5}$$

L'introduction de l'onde de contact stationnaire (valeur propre nulle associée au champ A) peut entraîner l'apparition du phénomène de résonance par chevauchement de ce champ linéairement dégénéré avec une onde vraiment non-linéaire.

Les deux techniques ci-dessus ont été appliquées et comparées sur un modèle simple d'écoulement diphasique dont le système d'équations est le suivant :

$$\partial_t (\rho\alpha) + \partial_x (\rho\alpha u) = \rho \frac{\alpha_{eq} - \alpha}{\tau_0} \tag{1.6}$$

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \tag{1.7}$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P(\rho)) = 0 \tag{1.8}$$

Les variables de ce système sont la densité moyenne du mélange ρ , la vitesse moyenne du mélange u et le titre du mélange α . Nous avons choisi une loi d'état simple de type "stiffened gas" ne dépendant pas du titre du mélange. De plus le titre à l'équilibre α_{eq} ainsi que le temps de relaxation τ_0 seront supposés constants et uniformes. Ce cadre simplifié a l'avantage de permettre de calculer des solutions analytiques.

La comparaison des deux techniques a été effectuée sur des cas tests simples et en faisant varier le temps de relaxation. Ce dernier permet de raidir le terme source et de tester les méthodes en régime plus ou moins fortement instationnaire. Les comportements observés semblent conformes à ce que l'on attendait. Les schémas de type "décentrement" perdent en précision lorsque le régime devient fortement instationnaire.

Chapitre 3 : Couplage interfacial des modèles des équations d'Euler en configuration isentropique à une et deux dimensions d'espace

La figure (1.2) représente un choix de modèles pour les différentes parties du circuit primaire d'une centrale. Ce choix implique de savoir coupler deux modèles dont les équations s'expriment dans des dimensions d'espace différentes, par exemple au niveau du raccord entre la cuve dans laquelle on applique un modèle tri-dimensionnel et le tuyau de sortie de cuve pour lequel on a choisi une modélisation mono-dimensionnelle. Ce chapitre présente une méthode permettant de coupler une cuve bi-dimensionnelle et un tuyau mono-dimensionnel. Il est important de noter qu'il n'y a aucune difficulté technique supplémentaire à traiter une cuve en trois dimensions, en revanche les coûts de calcul beaucoup plus importants limiteraient fortement l'étude sur maillages fins.

Afin de nous concentrer sur les problèmes liés aux dimensions d'espace, les modèles à coupler ne différeront que de ce point de vue. Les systèmes d'équations de part et d'autre de l'interface de couplage sont composés des équations isentropiques d'Euler auxquelles on adjoint une loi de fermeture thermodynamique simple de type "stiffened gas" :

$$P = s_0 \rho^\gamma - P_\infty, \quad \gamma > 1$$

où P désigne la pression et ρ la densité; s_0 et γ sont des paramètres. Cette équation d'état a l'avantage de permettre de simuler des écoulements de gaz (avec $P_\infty = 0$ on retrouve la loi des gaz parfaits) et d'obtenir une bonne approximation du comportement du liquide. Un travail analogue présenté en annexe B a été mené sur le système complet d'Euler, il est par ailleurs montré comment les méthodes proposées peuvent être étendues à plusieurs modèles basés sur le système des équations d'Euler.

Sans perte de généralité, les interfaces de couplage seront supposées parallèles à l'axe des ordonnées ($0y$). Les systèmes d'équations à coupler s'écrivent donc respectivement pour le côté tuyau et le côté cuve:

$$\left\{ \begin{array}{l} \partial_t(\rho) + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + P(\rho)) = 0 \\ v(x,t) = 0 \end{array} \right. \quad \left\{ \begin{array}{l} \partial_t(\rho) + \partial_x(\rho u) + \partial_y(\rho v) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + P(\rho)) + \partial_y(\rho uv) = 0 \\ \partial_t(\rho v) + \partial_x(\rho uv) + \partial_y(\rho v^2 + P(\rho)) = 0 \end{array} \right. \quad (1.9)$$

La méthode de couplage utilisée est issue du formalisme proposé par A.Y. Leroux. On introduit une variable z stationnaire et caractéristique des deux domaines. Celle-ci prend la valeur 0 dans le tuyau et 1 dans la cuve. Un modèle père, construit grâce à cette nouvelle variable, est introduit afin de calculer les flux de couplage au niveau de l'interface de couplage. Un calcul simple montre qu'il est nécessaire (et suffisant) que le flux calculé à l'aide du modèle père respecte une condition d'admissibilité. En effet, afin que la vitesse transverse v reste nulle dans le tuyau, le flux sur la composante transverse ρv doit être nul du côté du tuyau. Deux modèles admissibles ont été envisagés. Le premier est basé sur un système d'équations conservatives et donc assure la continuité des flux de couplage à travers l'interface de couplage, nous l'appellerons donc "modèle conservatif admissible" :

$$\partial_t(\rho) + \partial_x(\rho u) = 0 \quad (1.10)$$

$$\partial_t(\rho u) + \partial_x(\rho u^2 + P(\rho)) = 0 \quad (1.11)$$

$$\partial_t(\rho v) + \partial_x(z\rho uv) = 0 \quad (1.12)$$

En revanche, le deuxième système d'équations n'est que partiellement conservatif, il sera appelé "modèle non-conservatif admissible" :

$$\partial_t(\rho) + \partial_x(\rho u) = 0 \quad (1.13)$$

$$\partial_t(\rho u) + \partial_x(\rho u^2 + P(\rho)) = 0 \quad (1.14)$$

$$\partial_t(v) + zu\partial_x(v) = 0 \quad (1.15)$$

Ce système étant non-conservatif, la résolution du problème de Riemann associé n'est pas classique.

Afin d'étudier le comportement de chacun des modèles d'interface *d'un point de vue numérique*, différents tests ont été effectués sur la base de problèmes de Riemann déclenchés dans la cuve. La solution analytique d'un tel problème n'est malheureusement pas connue, et une solution numérique sur maillage fin fait office de solution de référence. Différents points ont été plus particulièrement examinés :

- la sensibilité aux coefficients de la loi thermodynamique, simulation en "eau" ou en gas.
- la sensibilité à la position de l'interface de couplage.

La comparaison entre le modèle conservatif et non-conservatif montre un meilleur comportement de ce dernier. Pour le premier, la pollution liée au couplage est en effet concentrée au niveau de l'interface de couplage. Dans le cadre du système complet des équations d'Euler (voir Annexes) ce phénomène conduit même à l'arrêt du calcul suite à l'apparition de valeurs discrètes négatives pour la densité. En revanche, dans le cadre de notre étude, les résultats relatifs des deux modèles ne semblent pas sensibles aux choix des coefficients thermodynamiques γ et P_∞ . La comparaison de différentes positions de l'interface de couplage confirme ce que l'on pouvait intuitivement espérer. En effet la pollution générée par les méthodes de couplage est moins importante lorsque l'interface de couplage est placée à l'intérieur du tuyau. En procédant ainsi, l'onde qui impacte l'interface de couplage a une amplitude moins grande en terme de vitesse transverse v : en pénétrant dans le tuyau l'écoulement se "redresse" et la composante transverse de la vitesse tend donc à s'évanouir.

Une annexe est dévolue à l'application de ces méthodes au cas du système des équations d'Euler incluant l'équation de bilan d'énergie totale. Il est par ailleurs montré que l'on peut aussi les étendre aux modèles homogènes relaxés ainsi qu'à un modèle simple prenant en compte la turbulence. Dans le cadre du système des équations d'Euler complet, les méthodes présentées ci-dessus permettent d'envisager de coupler des modèles possédant en outre une loi thermodynamique différente.

Chapitre 4 : Une méthode pour coupler deux modèles diphasiques homogènes de thermohydraulique nucléaire

Ce chapitre est consacré au couplage de deux modélisations différentes d'un écoulement diphasique. Les deux modèles choisis sont issus d'une représentation moyennée du mélange des phases liquide et vapeur, ils dérivent tous deux du modèle standard bi-fluide à une pression. La principale différence entre les deux modélisations est la manière dont est prise en compte le titre masse de liquide C .

Dans le premier modèle la variable C respecte une loi d'évolution, en temps et en espace, dictée par une équation aux dérivées partielles avec un terme source de retour à l'équilibre (Modèle Homogène Relaxé dénoté grâce à son acronyme anglais HRM). Le système d'équations associé au modèle HRM est :

$$\begin{cases} \partial_t(\rho C) + \partial_x(\rho CU) = \rho\Gamma(P, \rho, C) \\ \partial_t(\rho) + \partial_x(\rho U) = 0 \\ \partial_t(\rho U) + \partial_x(\rho U^2 + P) = 0 \\ \partial_t(\rho E) + \partial_x(U(\rho E + P)) = 0 \end{cases} \quad (1.16)$$

avec $E = e_{HRM}(P, \rho, C) + \frac{U^2}{2}$. Ce système est complété grâce à une loi de fermeture et un terme source Γ directement inspirés de ceux du code FLICA IV (voir ci-dessus). Pour le deuxième modèle, la grandeur C respecte un équilibre thermodynamique instantané la reliant à la pression P et la densité moyenne ρ (Modèle Homogène Equilibré dénoté grâce à son acronyme anglais HEM). Le système d'équations associé au modèle HEM est :

$$\begin{cases} \partial_t(\rho) + \partial_x(\rho U) = 0 \\ \partial_t(\rho U) + \partial_x(\rho U^2 + P) = 0 \\ \partial_t(\rho E) + \partial_x(U(\rho E + P)) = 0 \end{cases} \quad (1.17)$$

avec $E = e_{HEM}(P, \rho) + \frac{U^2}{2}$. Ce système est quant à lui complété grâce à une loi de fermeture inspirée de celle du code THYC (voir ci-dessus). Dans ce modèle, le titre masse liquide est donné par la

relation $C = C_{eq}(P, \rho)$.

Deux simplifications ont été faites par rapport aux codes THYC et FLICA IV. Nous avons considéré que les phases liquide et vapeur suivaient des *lois d'état de type gaz parfait*. De plus, la définition des *courbes de saturation en enthalpie a été simplifiée*. Celles-ci ont été choisies linéaires en pression, en revanche les coefficients de ces droites sont calculés à l'aide des tables thermodynamiques réelles THETIS. Cette simplification permet l'étude de certaines propriétés.

En réécrivant les différentes fermetures, deux relations de compatibilité entre ces deux modèles apparaissent. Toutes deux assurent que lorsque le modèle HRM est à l'équilibre il coïncide exactement avec le modèle (équilibré) HEM. Ces relations sont :

$$\Gamma(P, \rho, C_{eq}(P, \rho)) = 0$$

et

$$e_{HRM}(P, \rho, C_{eq}(P, \rho)) = e_{HEM}(P, \rho)$$

La technique de couplage qui a été mise en oeuvre s'inspire de la technique proposée par J.M. Greenberg et A.Y. Leroux. Cette technique a en effet l'inconvénient d'introduire une discontinuité stationnaire qui peut, dans certains cas, à des phénomènes de résonance. Afin d'éviter ce problème théoriquement mal appréhendé, il a été proposé notamment par F. Coquel de remplacer cette onde stationnaire par un champ *linéairement dégénéré* puis d'effectuer une étape de relaxation instantanée destinée à corriger les effets liés à l'étape de convection. Il reste alors à donner la valeur propre associée à ce champ linéairement dégénéré supplémentaire. Une idée naturelle consiste à s'appuyer sur le champ linéairement dégénéré préexistant associé aux ondes matérielles du modèle HEM et HRM, soit : $\lambda = U$. En effet, tout comme pour le système "classique" des équations d'Euler, les systèmes liés aux modèles HEM et HRM possèdent des valeurs propres ordonnées, les ondes rapides se trouvant de part et d'autre des ondes de matière.

La méthode numérique a été testée en se focalisant sur des problèmes de Riemann simples. Afin de se faire une idée du comportement du schéma d'interface, sa réponse au passage d'ondes simples a été regardée. Plusieurs paramètres sont pris en compte :

- la nature de l'onde émise allant interagir avec l'interface de couplage des codes : onde de choc, onde de détente ou discontinuité de contact ;
- le temps de relaxation du terme source Γ , gouvernant la "vitesse" de retour à l'équilibre du modèle HRM ;
- la finesse du maillage, qui comprend un maillage de taille "industriel" de 100 mailles, un maillage "fin" comprenant 10000 cellules, ainsi qu'un maillage intermédiaire de 500 mailles.

Les résultats obtenus sont comparés aux simulations fournies par les modèles HEM et HRM seuls sur l'ensemble du domaine sur maillage fin (qui jouent le rôle de solutions de référence) et sur maillage grossier (solutions de type industrielles). La notion d'erreur commise est ici plus conjecturale, ce qui n'était pas le cas dans le cadre du couplage du chapitre 3.

Ces résultats numériques montrent un bon comportement de la méthode de couplage. Les ondes de contact sont transmises sans aucune pollution lorsque celle-ci vont du domaine HEM vers le domaine HRM, en revanche le passage de ces ondes du modèle HRM vers le modèle HEM engendre des ondes parasites. Les ondes rapides sont quant à elles toujours à l'origine de pollution. Celle-ci reste néanmoins stable et d'amplitude raisonnable au moins sur les maillages les plus grossiers. Le

paramètre de relaxation du terme source Γ joue un rôle très important, en effet lorsque celui-ci est trop grand les solutions fournies par le modèles HRM sont trop dissemblables à celles fournies par le modèles HEM ; le couplage des deux modèles perd alors de son sens bien que la méthode soit en mesure de fournir un résultat.

Chapitre 5 : Couplage interfacial d'un modèle homogène et d'un modèle bi-fluide

La méthode proposée au chapitre précédent permet de coupler des modèles de thermo-hydraulique diphasique homogénéisés (HEM, HRM). Cette classe de modèles est largement utilisée dans le domaine de la simulation des écoulements diphasiques dans le milieu du nucléaire civil. Une autre classe de modèles est aussi largement utilisée ; il s'agit des modèles bi-fluides (modèle bi-fluide standard à une pression, modèle bi-fluides à deux pressions). Alors que les systèmes d'équations des modèles homogénéisés portent sur des grandeurs moyennées sur les deux phases, les systèmes d'équations des modèles bi-fluides portent sur des grandeurs phasiques. Pour ces derniers l'échange d'information entre les deux phases est assuré par des grandeurs interfaciales intervenant dans des termes non-conservatifs d'ordre un, ainsi que par les termes sources.

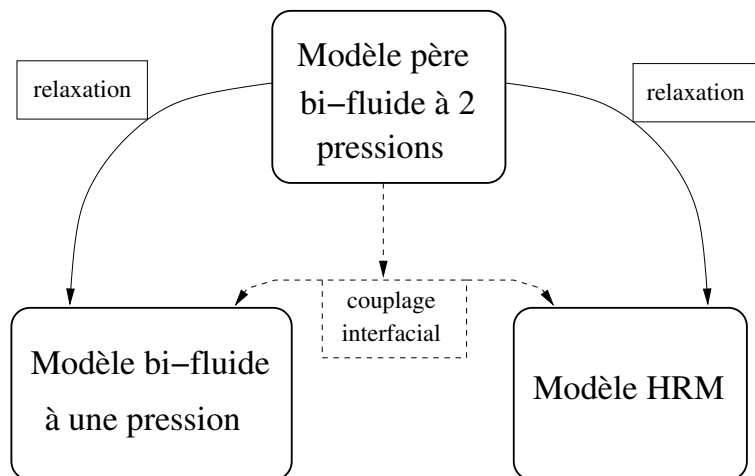


FIG. 1.3 – Le modèle bi-fluide à deux pressions est utilisé à la fois pour calculer des approximations du modèle HRM et du modèle bi-fluide standard à une pression, et pour assurer le couplage interfacial entre ces deux modèles.

Le couplage de deux modèles appartenant chacun à une de ces deux classes représente un enjeu majeur dans le cadre du projet NEPTUNE. Ce chapitre est consacré à l'adaptation de la méthode de couplage décrite au chapitre 4 au cas du couplage d'un modèle HRM (quatre équations) et du modèle bi-fluide standard à une pression (six équations). Ce couplage est réalisé grâce au modèle père (huit équations) construit sur la base du modèle bi-fluide standard à deux pressions (sept équations). Ce dernier est utilisé à la fois pour le calcul des flux de couplage et pour le calcul des approximations des solutions de chacun des deux modèles à coupler (comme l'indique la figure (1.3)).

La simulation numérique des modèles HRM et bi-fluide standard à une pression est réalisée grâce

à des méthodes de relaxation. La simulation du modèle bi-fluide standard à une pression est décrite dans l'annexe C. Une technique similaire est proposée pour calculer des approximations du modèle HRM à partir du modèle bi-fluide à deux pressions.

Les flux de couplage sont calculés grâce au modèle père basé sur le modèle bi-fluide à deux pressions. Le système d'équations associé à celui-là est le suivant :

$$\begin{cases} \partial_t (Y) = 0 \\ \partial_t (\alpha_l) + V_I \partial_x (\alpha_l) = \mathcal{A} \\ \partial_t (\alpha_l \rho_l) + \partial_x (\alpha_l \rho_l U_l) = \Gamma \\ \partial_t (\alpha_l \rho_l U_l) + \partial_x (\alpha_l \rho_l U_l^2 + \alpha_l P_l) - P_I \partial_x (\alpha_l) = \Psi_{3,l}(Y) \\ \partial_t (\alpha_l E_l) + \partial_x (\alpha_l U_l (E_l + P_l)) + P_I \partial_t (\alpha_l) = \Psi_{4,l}(Y) \\ \partial_t (\alpha_v \rho_v) + \partial_x (\alpha_v \rho_v U_v) = -\Gamma \\ \partial_t (\alpha_v \rho_v U_v) + \partial_x (\alpha_v \rho_v U_v^2 + \alpha_v P_v) - P_I \partial_x (\alpha_v) = -\Psi_{3,l}(Y) \\ \partial_t (\alpha_v E_v) + \partial_x (\alpha_v U_v (E_v + P_v)) + P_I \partial_t (\alpha_v) = -\Psi_{4,l}(Y) \end{cases} \quad (1.18)$$

où les variables sont :

- la variable domaine Y qui prend les valeurs 0 dans le domaine du modèle bi-fluide standard et 1 dans le domaine correspondant au modèle HRM ;
- les fractions volumiques des phases liquide α_l et vapeur α_v , reliées par la relation $\alpha_l + \alpha_v = 1$;
- les densités des phases liquide ρ_l et vapeur ρ_v ;
- les vitesses des phases liquide U_l et vapeur U_v ;
- les pressions au sein des phases liquide P_l et vapeur P_v .

Par ailleurs les énergies totales phasiques E_l et E_v s'expriment en fonction des énergies internes e_v et e_l ainsi que des énergies cinétiques phasiques :

$$E_\phi = \rho_\phi e_\phi(P_\phi, \rho_\phi) + \rho_\phi \frac{U_\phi^2}{2}, \quad \phi = v, l$$

La loi thermodynamique de chacune des phases est choisie dans la classe des gaz raides, c'est-à-dire que l'énergie interne s'écrit sous la forme :

$$(\gamma_\phi - 1) \rho_\phi e_\phi = P_\phi + \gamma_\phi P_{\infty, \phi}, \quad \phi = v, l \quad (1.19)$$

Une différence essentielle par rapport au couplage décrit au chapitre 4 est la suivante : dans la partie convective du système (1.18) la variable Y n'intervient que dans la première équation. Ceci est dû au fait que les deux modèles à coupler sont obtenus en relaxant les équations du même modèle père, ce qui assure implicitement la compatibilité des relations de fermeture thermodynamique des deux modèles. De plus, le champ associé à la variable Y est un champ linéairement dégénéré stationnaire. La structure propre du système (1.18) ne dépendant pas de Y , cette onde stationnaire ne sera pas à l'origine de phénomène de résonance.

Le choix du modèle bi-fluide à deux pressions comme modèle de base nous permet de travailler avec un système qui a l'avantage d'être inconditionnellement hyperbolique, ce qui n'est pas le cas du modèle bi-fluide standard. De plus, avec un choix judicieux des lois de fermeture, la fermeture des relations de saut est unique malgré la présence de termes non-conservatifs.

Les tests numériques ont été effectués sur des problèmes de Riemann mono-dimensionnels et bi-dimensionnels. Il s'avère que la méthode est stable et que l'amplitude des ondes réfléchies reste faible

relativement aux ondes générées par la discontinuité des données initiales. De plus aucune pollution stationnaire n'est visible au niveau de l'interface de couplage; ceci est dû à la forte compatibilité entre les deux modèles couplés.

Chapitre 2

Étude comparative de schémas numériques pour les systèmes hyperboliques avec termes sources en régime instationnaire

Dans les modèles servant à simuler les écoulements diphasiques dans les circuits hydrauliques des centrales nucléaires, les phénomènes de transfert de masse ou les effets de trainée et de portance entre les phases sont pris en compte par des termes sources d'ordre zéro. Ceux-ci jouent un rôle fondamental pour le respect de la physique de l'écoulement ; et en pratique se pose le problème de la prise en compte numérique de ces termes sources. En gardant un cadre général les systèmes hyperboliques avec termes sources d'ordre zéro s'écrivent sous forme "conservative" de la façon suivante :

$$\partial_t (W) + \partial_x (F(W)) = S(W) \quad (2.1)$$

où W est le vecteur rassemblant les variables conservatives du système, $W \mapsto F(W)$ est le flux analytique et où $W \mapsto S(W)$ représente les termes sources.

Ce chapitre est dévolu à l'étude comparative de deux approches fondamentalement différentes de prise en compte des termes sources. La première est la plus intuitive et la plus utilisée, surtout dans le milieu des codes industriels. Il s'agit de la méthode à pas fractionnaires [80]. Cette méthode décompose le système d'équations aux dérivées partielles (2.1) en deux systèmes traités l'un après l'autre. La première étape consiste à traiter la partie convective de (2.1) (i.e. on pose formellement $S(W)=0$) tandis que la deuxième étape se focalise sur le système dynamique lié aux termes sources :

$$\partial_t (W) = S(W) \quad (2.2)$$

Le traitement dissocié des phénomènes de convection et des termes sources pose néanmoins problème lorsque l'on se trouve dans un régime de fonctionnement stationnaire, $\partial_t W = 0$. En effet dans de telles situations, l'équilibre $\partial_x F(W) = S(W)$ entre la partie convective du système et les termes sources peut échapper au schéma numérique de type pas fractionnaires sur maillages grossiers. C'est dans l'optique de respecter de telles solutions qu'ont été introduits les "schémas équilibre" [67], [44] ou [73]. L'idée est d'intégrer les termes sources à la partie convective du système. Le traitement des

termes sources est donc décentré au niveau des interfaces entre les cellules. Pour cela on introduit une variable $a(x,t)$ telle que $\partial_x a = 1$ et $\partial_t a = 0$. Le système permettant le calcul des flux aux interfaces est alors :

$$\begin{cases} \partial_t (a) = 0 \\ \partial_t (W) + \partial_x (F(W)) - S(W)\partial_x (a) = 0 \end{cases} \quad (2.3)$$

Les systèmes du type de (2.3) ne sont pas des systèmes hyperboliques classiques. En effet, outre les problèmes liés à la définition du produit non-conservatif $S(W)\partial_x a$, l'introduction du champ linéairement dégénéré associé à la valeur propre 0 peut engendrer des problèmes de résonance.

L'étude sera faite sur un modèle simplifié d'écoulement diphasique basé sur les équations isentropiques d'Euler auxquelles on adjoint une équation de transport d'un titre avec en second membre un terme source de retour à l'équilibre. Ce terme de relaxation ne porte que sur le titre et est piloté par un temps de relaxation τ_0 supposé constant et uniforme, de même la valeur du titre à l'équilibre α_{eq} sera constante et uniforme. Le système s'écrit :

$$\begin{cases} \partial_t (\rho\alpha) + \partial_x (\rho\alpha u) = \rho \frac{\alpha_{eq} - \alpha}{\tau_0} \\ \partial_t (\rho) + \partial_x (\rho u) = 0 \\ \partial_t (\rho u) + \partial_x (\rho u^2 + P(\rho)) = 0 \end{cases} \quad (2.4)$$

Nous avons choisit une loi d'état de type gaz parfait, portant sur la pression P , et qui ne dépend pas du titre α mais uniquement de la densité ρ . Ainsi on est en mesure d'explicitier la solution analytique d'un problème de Riemann pour le système (2.4) et ainsi de calculer des ordres de convergence pour les schémas numériques. De plus, en jouant sur le temps de relaxation τ_0 on pourra tester les différents schémas numériques dans des configurations plus ou moins stationnaires.

En plus du schéma à pas fractionnaires (abréviation S_{FS}) et du schéma de décentrement classique (abréviation S_{UPW1}) nous proposons un deuxième schéma de décentrement (abréviation S_{UPW2}). Pour le schéma S_{UPW2} le calcul des flux est le même que pour le schéma S_{UPW1} , les deux utilisent le même modèle d'interface. En revanche le schéma S_{UPW1} utilise un schéma de maille (i.e. bilan des flux pour calculer les valeurs de maille) classique basé sur les variables conservatives $\rho\alpha$, ρ et ρu , tandis que le schéma S_{UPW2} utilise un schéma de maille basé sur les variables ρI , ρ et ρu où la variable $I = a + u\Phi$ est un invariant de Riemann pour l'onde stationnaire (i.e. associée à la valeur propre 0). Cette modification apporte une amélioration sensible des résultats du schéma de décentrement en régime instationnaire.

Dans l'optique du couplage interfacial de modèles différents en *régime instationnaire*, les résultats de nos tests numériques nous montrent que la stratégie liée au schéma S_{UPW1} n'est pas optimale. Il s'avère ici que le comportement du schéma S_{FS} est toujours satisfaisant surtout pour les régimes fortement instationnaires. De plus sa simplicité de mise en oeuvre nous conduit à le préférer au schéma S_{UPW2} , surtout dans un cadre industriel complexe tel que le cas décrit au chapitre 4.

Well balanced schemes versus fractional step method for hyperbolic systems with source terms

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Abstract : The paper is devoted to the analysis of the real accuracy of different schemes when computing a simple hyperbolic model with source terms, which describes the motion of two-phase flows including source terms. The strategy of upwinding the source terms is investigated and compared with the standard fractional step method. A first scheme relies on the usual fractional step approach. A second scheme applies for upwinding of source terms. This one however does not provide satisfactory results when computing some specific *unsteady* cases. This behavior can be easily explained. It thus motivates to introduce a third scheme, which is similar to the previous one but aims at providing an increased accuracy on coarse meshes when computing highly unsteady flows. This latter scheme requires to define a cell scheme which computes the void fraction with help of a modified governing equation, while using the same interface solver. A detailed numerical study which includes a measure of the L^1 norm of the error completes the whole.

2.1 Introduction

A first result for the discretization of source terms for hyperbolic conservation laws was given by Roe in 1986 [66], introducing the idea of upwinding of source terms. Afterwards, an extensive literature has been devoted to the numerical treatment of steady states with well balanced schemes, following ideas introduced by Greenberg and Leroux [44] (see [41],[42], [43], [67] too). The main objective in these well-balanced schemes is to preserve steady solutions on coarse meshes. In particular, it has been successfully used to deal with shallow water equations with topography, or similarly to handle one dimensional Euler steady computations in nozzles (see [33] and [58] for instance). It has also been checked that the well-balanced schemes enable to reach a steady state, as a limit for large time, of an unsteady solution. The basic idea is roughly the following: if source terms exactly balance convective effects, source terms have to be upwinded in accordance with upwinded convective fluxes.

Owing to this great success, it also seems appealing to use the well-balanced schemes to compute unsteady flows, and meanwhile benefit from the previous properties for large time. We show here, on the basis of particular initial conditions for a given system (which contains a relaxation time in the source term), that the unsteady approximation predicted by the well-balanced scheme may be far less accurate than the one given for instance by the standard fractional step method ([80]), although both of them converge towards the same solution, as the mesh size vanishes, and with the same rate of convergence. Actually, depending on the system and its initial conditions, there may be a balance between the time derivative and the source term, or a balance between the space derivative and the time derivative, depending on (x,t) .

In order to investigate the true accuracy of the fractional step method and the methods involving an upwinding of source terms when computing *unsteady* solutions, we will focus on a particular model. The model which will be examined herein is a three-equation model, and it issues from the two-phase flow framework. This model contains a source term which accounts for mass transfer between phases. The source term represents a relaxation term to some thermodynamical equilibrium. The associated relaxation time essentially depends whether one accounts for condensation, flashing or evaporation effects. As a consequence, the stiffness of source terms is variable, and may be dominant over convective effects, or on the contrary be completely negligible. This kind of source should not be confused with other sources such as effects of topography in shallow water equations, which do not involve external time scales.

Once the model is introduced, we will focus on three distinct schemes :

- the first scheme relies on the well-known fractional step approach, and it simply consists in two steps. In the first step, advective terms are accounted for, whereas in the second step, (possibly stiff) source terms are approximated. The main advantages are the following. The resulting scheme is much stable; one may apply "standard" hyperbolic schemes to discretize first-order terms; eventually, this decouples effects so that users who are not familiar with upwinding techniques may concentrate on the sources,
- the second scheme is the classical well-balanced scheme, which has been introduced some time ago in order to compute *steady* nonhomogeneous hyperbolic systems. Source terms are "upwinded", in order to represent steady states on coarse meshes in a very accurate way. This has been motivated by the rather poor behaviour (more precisely the poor accuracy) of the fractional step approach (noted S_{FS} afterwards) in steady situations.

- the third scheme is a new scheme. It is based on a slight modification of the standard well-balanced scheme, and it involves a modification of the unknowns which are computed.

All cell schemes and interface solvers will be detailed. Interface solvers rely on the approximate Godunov approach ([16], [31]), but we insist that conclusions would be the same if one uses the exact Godunov scheme ([40]) instead. The measure of the L^1 norm of the error in *unsteady* test cases enables to get a precise idea of true advantages and drawbacks of the three schemes.

It will clearly appear that none among the two strategies may be disregarded, since:

- (i) the fractional step method behaves rather well in all *unsteady* situations on coarse meshes,
- (ii) the upwind approach should be preferred when *steady* approximations are searched on coarse meshes,
- (iii) a slight modification of well-balanced schemes may drastically improve the accuracy of approximations of unsteady solutions on coarse meshes.

2.2 A simplified model to describe two-phase flows

We consider a simple two-phase flow model which describes the motion of a mixture including two components with mass transfer terms. The convective part of the model is in conservative form, and we define the conservative variable $W = {}^t(\rho, \rho\alpha, \rho u)$, where ρ stands for the mean density of the mixture, u is the mean velocity in the field, and α is the concentration of one component :

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (2.5)$$

$$\partial_t (\rho\alpha) + \partial_x (\rho\alpha u) = \rho s(\alpha) \quad (2.6)$$

$$\partial_t (\rho u) + \partial_x ((\rho u^2 + P(\rho))) = \partial_x ((\mu \partial_x (u))) \quad (2.7)$$

The source term s depends on α and involves some constant time scale τ_0 , μ is a positive constant, and the function $P(\rho)$ is increasing, and such that $P(0) = 0$. The homogeneous flux is $F(W) = (\rho u, \rho\alpha u, \rho u^2 + P(\rho))$.

The void fraction $\alpha(x,t)$ should lie in $[0,1]$. This will be referred to as the bound constraints in the following. In order to clarify the presentation, we will from time to time specify some form for the source term $s(\alpha)$, that is:

$$s(\alpha) = \frac{\alpha_{eq} - \alpha}{\tau_0}$$

with α_{eq} in $I_{adm} = [0,1]$. We now describe the entropy inequality which is valid for regular solutions.

Property 1

An entropy pair $(\eta(W), F_\eta(W))$ for the system (2.5)-(2.7) is ,

$$\begin{aligned} \eta(W) &= \frac{\rho u^2}{2} + \rho\psi_1(\rho) + \rho\psi_2(\alpha) \\ F_\eta(W) &= (\eta(W) + P(\rho))u \end{aligned}$$

with $\psi_1(\rho) = \int_0^\rho (\frac{P(a)}{a^2}) da$ and $\psi_2(\alpha) = -\int_0^\alpha s(a) da$. The entropy $\eta(W)$ is strictly convex with respect to W , if and only if $s'(\alpha) < 0$. The following entropy inequality holds for regular solutions of (2.5)-(2.7):

$$\partial_t (\eta(W)) + \partial_x (F_\eta(W)) - \partial_x ((\mu u \partial_x (u))) < -\rho s^2 \quad (2.8)$$

◇

Introducing as usual the speed of sound waves c as:

$$c(\rho) = (P'(\rho))^{1/2} \quad (2.9)$$

one may check that the homogeneous convective set (or left hand side) of system (2.5)-(2.7):

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (2.10)$$

$$\partial_t (\rho\alpha) + \partial_x (\rho\alpha u) = 0 \quad (2.11)$$

$$\partial_t (\rho u) + \partial_x ((\rho u^2 + P(\rho))) = 0 \quad (2.12)$$

is hyperbolic, since eigenvalues are real and distinct unless vacuum arises. Eigenvalues are:

$$\lambda_1 = u - c \quad (2.13)$$

$$\lambda_2 = u \quad (2.14)$$

$$\lambda_3 = u + c \quad (2.15)$$

Fields 1 and 3 are genuinely non linear, and the 2 field is linearly degenerated. The entropy inequality ensures that the jump of u is negative through shock waves: $u_r - u_l < 0$, if subscripts l, r respectively denote the states on the left and right side of the traveling shock wave.

Before going further on, we recall that the one dimensional Riemann problem corresponds to the initial value problem associated with the hyperbolic system:

$$\partial_t (W) + \partial_x (F(W)) = 0 \quad (2.16)$$

and the discontinuous initial data:

$$W(x, t = 0) = W_L \quad \text{if: } x < 0 \quad \text{and:} \quad W(x, t = 0) = W_R \quad \text{if: } x > 0 \quad (2.17)$$

Everywhere in the following of the manuscript, the subscripts L and R will refer to the left and right states of the initial condition W_L and W_R .

Within the class of self-similar functions $W(x, t) = w(x/t)$ composed of constant states separated by shock waves, rarefaction waves and contact discontinuities, the construction of the entropy-consistent solution of the one-dimensional Riemann problem associated with the set ((2.10),(2.12)) with no vacuum occurrence (i.e. $\rho > 0$) is classical, and thus is not recalled herein (see [75] for instance). Actually, the existence and uniqueness of this solution is ensured if and only if the initial data agrees with:

$$u_R - u_L < g(\rho_L) + g(\rho_R) \quad (2.18)$$

where:

$$g(\rho) = \int_0^\rho \frac{c(a)}{a} da. \quad (2.19)$$

In addition, the solution of the 1D Riemann problem is such that the bound constraints for the void fraction α are fulfilled. We only briefly recall the structure of the solution. The 1-wave and the 3- wave admit the following Riemann invariants:

$$I^1 = \{u + g(\rho), \alpha\}$$

and:

$$I^3 = \{u - g(\rho), \alpha\}$$

respectively. Besides, the Riemann invariants in the 2-wave are:

$$I^2 = \{u, P\}$$

An important point to note is that α may not vary in a 1-shock or in a 3-shock. As a consequence, the bound constraints for α cannot be violated.

Remark 1 *If the condition (2.18) is violated, a vacuum occurs in the solution, and the uniqueness of the solution (ρ, u) is no longer ensured. Actually, the definition of the velocity in the vacuum area no longer makes sense in that case (among others, one may refer to [21] for instance which details the construction of the solution (ρ, pu) in such a case).*

In the remaining of the paper , we will deal with non viscous flows $\mu = 0$.

We now introduce some function $A(x,t)$ such that $A(x,t = 0) = x$. We rewrite the governing equations (2.5)-(2.7) with $\mu = 0$ in the following form:

$$\partial_t (A) = 0 \quad (2.20)$$

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (2.21)$$

$$\partial_t (\rho \alpha) + \partial_x (\rho \alpha u) - \rho s \partial_x (A) = 0 \quad (2.22)$$

$$\partial_t (\rho u) + \partial_x ((\rho u^2 + P(\rho))) = 0 \quad (2.23)$$

The non conservative system (2.20)-(2.23) is hyperbolic, since eigenvalues are real and distinct:

- $\lambda_1 = 0$
- $\lambda_2 = u$
- $\lambda_3 = u - c$
- $\lambda_4 = u + c$

unless vacuum arises ($\rho = 0$), or if $u = 0$. Fields 3 and 4 are genuinely non linear, and the 1 and 2 fields are linearly degenerated. For convenience, we will use $Z = (A, \alpha, \rho, u)$. Regular solutions of the previous system are governed by:

$$\partial_t (A) = 0 \quad (2.24)$$

$$\partial_t (\alpha) + u \partial_x (\alpha) - s(\alpha) \partial_x (A) = 0 \quad (2.25)$$

$$\partial_t (\rho) + u \partial_x (\rho) + \rho \partial_x (u) = 0 \quad (2.26)$$

$$\partial_t (u) + u \partial_x (u) + \frac{P'(\rho)}{\rho} \partial_x (\rho) = 0 \quad (2.27)$$

or in a condensed form: $\partial_t (Z) + C(Z) \partial_x (Z) = 0$. The fields labeled 1 and 2 are linearly degenerated and the Riemann invariants associated with the 1-wave and the 2-wave are:

- $J^1 = \{u, \rho, A + u\phi(\alpha)\}$
- $J^2 = \{u, \rho, A\}$

where ϕ is defined for $s(\alpha) \neq 0$ as:

$$\phi'(\alpha) = -\frac{1}{s(\alpha)} \quad (2.28)$$

The fields labeled 3 and 4 are genuinely non linear and the Riemann invariants associated with the 3-wave and the 4-wave are:

- $J^3 = \{u + g(\rho), \alpha, A\}$
- $J^4 = \{u - g(\rho), \alpha, A\}$

In the limit case where $u = 0$, the sets J^1 and J^2 coincide.

We now introduce a few notations on figures (2.1) and (2.2) depending whether the speed of the contact discontinuity associated with λ_2 is positive or negative respectively. We first detail the structure of the solution (ρ, u) in the one-dimensional Riemann problem.

- If $\lambda_2 > 0$, then, owing to J^1 and J^2 , and due to the fact that both the 1-wave and the 2-wave are linearly degenerated, we immediately get $u_{1,l} = u_{1,r} = u_{2,r} = u_1$ and $\rho_{1,l} = \rho_{1,r} = \rho_{2,r} = \rho_1$.
- If $\lambda_2 < 0$, for the same reasons , we get $u_{2,l} = u_{1,l} = u_{1,r} = u_1$ and $\rho_{2,l} = \rho_{1,l} = \rho_{1,r} = \rho_1$.

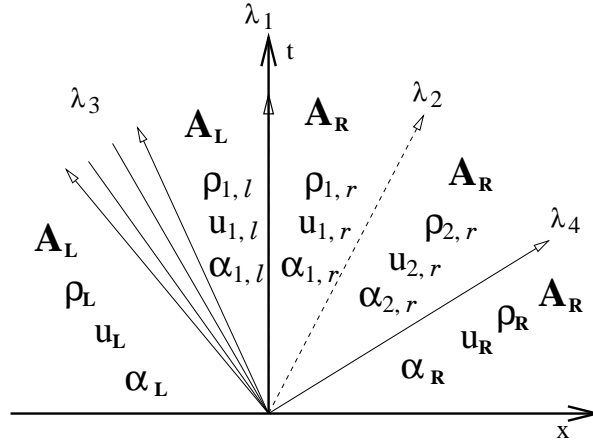


FIG. 2.1 – Structure of the solution of the one dimensional Riemann problem ($\lambda_2 > 0$)

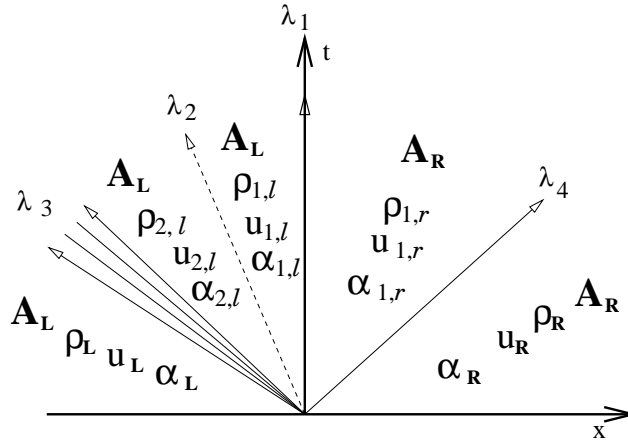


FIG. 2.2 – Structure of the solution of the one dimensional Riemann problem ($\lambda_2 < 0$)

Thus, u_1 and ρ_1 will respectively refer to the intermediate velocity and to the intermediate density between the genuinely non linear 3–wave and the genuinely non linear 4–wave, and we note $c_1 = c(\rho_1)$.

Proposition 2a

The one-dimensional Riemann problem associated with (2.21) and (2.23) has a unique entropy consistent solution (ρ, u) composed of constant states (ρ_L, u_L) , (ρ_1, u_1) , (ρ_R, u_R) separated by shock waves or rarefaction waves in the 3-wave and the 4-wave, with no vacuum occurrence, provided that the initial data $(\rho_L, u_L), (\rho_R, u_R)$ agrees with the following condition:

$$u_R - u_L < g(\rho_L) + g(\rho_R) \quad (2.29)$$

◇

This is a classical result ([37]).

In order to get some construction of the whole solution, we need to describe more accurately the form of the source term in order to compute the remaining unknown α . We will focus below on:

$$s(\alpha) = \frac{\alpha_{eq} - \alpha}{\tau_0}$$

but the proof that is given is obviously still valid when focusing on many other source terms. If one focuses on regular solutions of equation (2.25), we first note that it may be classically shown that bound constraints are satisfied (see for instance [34] which recalls this standard result). If one turns to solutions of the Riemann problem, we need the following new result:

Proposition 2b

We assume that the condition (2.29) holds. Then the bound constraints for the void fraction are guaranteed in the solution of the one dimensional Riemann problem associated with ((2.20) - (2.23)), which means that the solution $\alpha(x,t)$ of the Riemann problem lies in I_{adm} .

◇

Proof:

– Part I:

We will first focus on the case where the intermediate state u_1 is strictly positive.

In that case, the 3–wave may either behave:

- (i) as a subsonic 3–rarefaction wave which spans in $(x < 0, t > 0)$, when $u_1 - c_1 < 0$;
- (ii) or as a supersonic 3–rarefaction wave which overlaps $x/t = 0$, when $u_L - c_L < 0$ and $u_1 - c_1 > 0$;
- (iii) or as a supersonic 3–rarefaction wave which spans in $(x > 0, t > 0)$, when $u_L - c_L > 0$;
- (iv) or as a left going 3–shock wave of speed σ_3 ;
- (v) or as a right going 3–shock wave of speed σ_3 .

In situations (i) and (iv), the velocity along $x/t = 0$ is $u_{x=0} = u_1$, whereas in case (iii) and (v), it reads $u_{x=0} = u_L$. The last possibility is $u_{x=0} = c_{x=0}$ if (ii) occurs. In situations (i), (ii), (iii) and (iv), one thus obtains $u_{x=0} > 0$. Making use of Lax inequality, we also check that $u_L - c_L > \sigma_3$ in situation (v), which immediately turns into $u_{x=0} = u_L > \sigma_3 + c_L > 0$. Hence in all cases, we get $u_{x=0} > 0$.

The solution is such that: $\alpha_{1,l} = \alpha_L$ and $\alpha_{2,r} = \alpha_R$, owing to J^3 and J^4 , and to the fact that the void fraction α does not vary through 3 – 4-shock waves. The remaining unknown is $\alpha_{1,r}$ (see figure (2.1)):

$$\alpha(x/t) = \alpha_L \quad \text{if } x/t < 0 \tag{2.30}$$

$$\alpha(x/t) = \alpha_{1,r} \quad \text{if } 0 < x/t < u_1 \tag{2.31}$$

$$\alpha(x/t) = \alpha_R \quad \text{if } x/t > u_1 \tag{2.32}$$

Thus, it only remains to prove that $\alpha_{1,r}$ lies in the admissible range. The solution $\alpha_{1,r}$ fulfills:

$$A_R + u_{x=0}\phi(\alpha_{1,r}) = A_L + u_{x=0}\phi(\alpha_L) \tag{2.33}$$

and is thus the solution of the equation:

$$f(\alpha) = \frac{A_R - A_L}{u_{x=0}} + \phi(\alpha) - \phi(\alpha_L) = 0 \tag{2.34}$$

where $A_R - A_L = h$. It remains to check that $\alpha_{1,r}$ belongs to $[0,1] - \{\alpha_{eq}\}$.

We introduce now $s(\alpha) = \frac{\alpha_{eq} - \alpha}{\tau_0}$. We thus get $f'(\alpha) = \phi'(\alpha) = \frac{-1}{s(\alpha)} = \frac{\tau_0}{\alpha - \alpha_{eq}}$. Thus:

- If $\alpha_L > \alpha_{eq}$, the unique solution will be :

$$\alpha_{1,r} = \alpha_{eq} + e^{-\frac{h}{\tau_0 u_{x=0}}} (\alpha_L - \alpha_{eq}) \quad (2.35)$$

By the way we note that $\alpha_{1,r}$ tends towards α_{eq} when $u_{x=0}$ tends towards 0^+ , whatever the mesh size is.

- If we turn now to the case where $\alpha_L < \alpha_{eq}$, the unique solution of equation (2.34) is again (2.35). It may be checked that the solution $\alpha_{1,r}$ lies in (α_L, α_{eq}) in any case.

- *Part II:*

In a similar way, we may investigate the case $u_1 < 0$.

This leads to the same discussion. Since $\alpha_{2,l} = \alpha_L$ and $\alpha_{1,r} = \alpha_R$, the remaining unknown is now: $\alpha_{1,l}$ (see figure (2.2)). This eventually provides the solution

$$\alpha(x/t) = \alpha_L \quad \text{if } x/t < u_1 \quad (2.36)$$

$$\alpha(x/t) = \alpha_{1,l} \quad \text{if } u_1 < x/t < 0 \quad (2.37)$$

$$\alpha(x/t) = \alpha_R \quad \text{if } x/t > 0 \quad (2.38)$$

where $\alpha_{1,l}$ is now :

$$\alpha_{1,l} = \alpha_{eq} + e^{\frac{h}{\tau_0 u_{x=0}}} (\alpha_R - \alpha_{eq}) \quad (2.39)$$

Note that $u_{x=0} < 0$ now. Thus the solution $\alpha_{1,l}$ now lies in (α_R, α_{eq}) , thus in I_{adm} . We still check that $\alpha_{1,l}$ tends towards α_{eq} when $u_{x=0}$ tends towards 0^- .

◇

2.3 Standard fractional step method (S_{FS})

We want to compute approximations of solutions of the following non-homogeneous system:

$$\begin{cases} \partial_t(W) + \partial_x(F(W)) = S(W) \\ W(x,0) = W_0(x) \end{cases}$$

using a fractional step method ([80]). Thus, at each time step, we compute W^{n+1} in terms of W^n , by solving:

$$\begin{aligned} (P1) & : \partial_t(W^\circ) + \partial_x(F(W^\circ)) = 0, W^\circ(x,0) = W^n(x) \\ (P2) & : \partial_t(W) = S(W), W(x,0) = W^\circ(x,\Delta t) \end{aligned}$$

successively.

The problem (P1) corresponds to the computation of approximations of solutions of (2.10)-(2.12) using the following classical scheme:

$$\Delta x((W_i^\circ)^{n+1} - W_i^n) + \Delta t(F(W_i^n, W_{i+1}^n) - F(W_{i-1}^n, W_i^n)) = 0$$

where $F(W_i^n, W_{i+1}^n)$ is a numerical flux, which depends on two states W_i^n and W_{i+1}^n . This numerical flux will be defined later on (see section 4 where the approximate Godunov scheme based on [16] will be detailed). At this stage, we want to emphasize that some properties of the whole scheme will be tightly linked with the choice of our interface solvers which will provide forms of numerical fluxes.

The problem (P2) requires to look for approximate solutions of the ordinary differential system:

$$\partial_t(\rho\alpha) = \rho s(\alpha) \tag{2.40}$$

$$\partial_t(\rho) = 0 \tag{2.41}$$

$$\partial_t(\rho u) = 0 \tag{2.42}$$

At each time step, (2.41) provides $\rho_i^{n+1} = (\rho_i^\circ)^{n+1}$ and (2.42) leads to $u_i^{n+1} = (u^\circ)^{n+1}$. Equation (2.40) is integrated in such a way that the lower and upper bounds of α^{n+1} are ensured. We will use an exact integration of (2.40) and (2.41) in our numerical tests.

In the remaining of the paper, this scheme will be referred to as S_{FS} .

2.4 Well-balanced schemes and interface Riemann solvers

2.4.1 Interface Riemann solvers

We still use notations (2.9), (2.19) and (2.28).

Our interface Riemann solvers will require to introduce a change of variable, so that we can work with the new variable $Y(W)$. Moreover, for given left and right states W_L and W_R in the initial condition, we will define some average \hat{Y} which will depend only on $Y_L = Y(W_L)$ and $Y_R = Y(W_R)$. Given that average \hat{Y} , obvious notations will be used which are: $\hat{\lambda}_k = \lambda_k(\hat{Y})$, $\hat{r}_k = r_k(\hat{Y})$, $\hat{u} = u(\hat{Y})$, $\hat{\rho} = \rho(\hat{Y})$, $\hat{c} = c(\hat{Y})$.

In practice, we will focus in this paper on the following classical choice (see [16]):

$$\hat{Y}_{LR} = (Y_L + Y_R)/2 \quad (2.43)$$

(other choices such as the one detailed in [29] might be considered).

We also denote for any quantity ϕ : $(\Delta\phi)_{LR} = \phi_R - \phi_L$ and $(\bar{\phi})_{LR} = (\phi_R + \phi_L)/2$. Moreover for any $k = 1..4$, $F_{k,l}$ (resp. $F_{k,r}$) denotes the value of F on the left (resp. right) side of the Linearly Degenerate field associated with the eigenvalue $\hat{\lambda}_k$.

Basic interface solver

The left hand side of system (2.24)-(2.27) may be rewritten in terms of the non conservative variable $Y(W) = {}^t(A, \phi, \rho, u)$ in the form:

$$\partial_t(Y) + C(Y)\partial_x(Y) = 0 \quad (2.44)$$

where:

$$C(Y) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & u & 0 & 0 \\ 0 & 0 & u & \rho \\ 0 & 0 & \frac{c^2}{\rho} & u \end{pmatrix}$$

We turn now to the associated linearized problem:

$$\partial_t(Y) + C(\hat{Y}_{LR})\partial_x(Y) = 0 \quad (2.45)$$

By denoting: $\hat{\lambda}_1 = 0$, $\hat{\lambda}_2 = \hat{u}$, $\hat{\lambda}_3 = \hat{u} - \hat{c}$, $\hat{\lambda}_4 = \hat{u} + \hat{c}$, the right eigenvectors \hat{r}_k associated with $\hat{\lambda}_k$ are respectively:

$$\hat{r}_1 = (\hat{u}, -1, 0, 0) \quad (2.46)$$

$$\hat{r}_2 = (0, 1, 0, 0) \quad (2.47)$$

$$\hat{r}_3 = (0, 0, \hat{\rho}, -\hat{c}) \quad (2.48)$$

$$\hat{r}_4 = (0, 0, \hat{\rho}, \hat{c}) \quad (2.49)$$

The inverse of the matrix of the right eigenvectors $r_k(Y)$ is $(2\rho cu)^{-1}\omega$, where ω stands for:

$$\begin{pmatrix} 2\rho c & 0 & 0 & 0 \\ 2\rho c & 2\rho cu & 0 & 0 \\ 0 & 0 & uc & -\rho u \\ 0 & 0 & uc & \rho u \end{pmatrix}$$

The computation of the intermediate states in the linearized solver at each interface between two cells labeled L, R is very easy (see [16] where the basis of the approximate Godunov scheme is recalled). Intermediate states for (ρ, u) components are given through (see figure (2.3) for notations):

$$\rho_1 = \bar{\rho}_{LR} - \frac{\hat{\rho}(\Delta u)_{LR}}{\hat{c}} \frac{1}{2} \quad \text{and} \quad u_1 = \bar{u}_{LR} - \frac{\hat{c}(\Delta \rho)_{LR}}{\hat{\rho}} \frac{1}{2}$$

A robust interface solver

We now consider the choice of the non-conservative variable $Y(W) = {}^t(A, \phi, g(\rho), u)$ in (2.44) and (2.45). The main advantage of the latter is that it enables to preserve positive values for the mean density:

Property:

No vacuum arises in the intermediate states of this linearized Godunov solver if and only if the initial data does not make vacuum occur in the exact solution of the Riemann problem associated with the non linear set of equations, that is if:

$$u_R - u_L < g_L + g_R \tag{2.50}$$

and if the following extra-condition holds:

$$\int_0^{+\infty} \left(\frac{c(a)}{a} da \right) = +\infty \tag{2.51}$$

The first part of the proof is given in [32]. It deeply relies on the fact that the Riemann invariants of the 3–field and the 4–field are linear with respect to $g(\rho)$ and u , and that the latter two are components of Y . Actually, as proved in [32], this enables to reproduce perfectly rarefaction waves through the approximate linearized solver.

The second extra-condition (2.51) is also due to the choice of the *approximate* Godunov scheme, since the latter no longer distinguishes shock waves from rarefaction waves, unlike Godunov scheme of course. The proof may be found in [29].

Before going further on, we emphasize that for standard EOS such as $P(\rho) = P_0 \rho^\gamma$ with $\gamma > 1$, we get $g(\rho) = 2c(\rho)/(\gamma - 1)$ with $c(\rho) = (\gamma P_0 \rho^{(\gamma-1)})^{1/2}$; thus, the extra condition (2.51) is obviously fulfilled.

We now give some details on the discrete values of the void fraction α .

On the preservation of bound constraints for the void fraction in the interface solvers

Both "basic and robust" interface solvers provide the same intermediate states of the void fraction which are defined as follows. These require to compute $\phi(\alpha)$ first.

The solution of the linear Riemann problem associated with (2.45) is classical. One simply needs to compute :

$$Y_{k,r} - Y_{k,l} = \beta_k \hat{r}_k \tag{2.52}$$

where the β_k issue from the decomposition of the difference $Y_R - Y_L$:

$$Y_R - Y_L = \sum_1^4 \beta_k \hat{r}_k \quad (2.53)$$

In order to achieve this, one has to use the forms of the right eigenvectors (2.46)-(2.49). Nonetheless, for convenience, one needs to distinguish here whether $\hat{u}_{LR} > 0$ or $\hat{u}_{LR} < 0$.

- If $\hat{u}_{LR} > 0$, left and right states of ϕ on each side of the steady contact discontinuity $\frac{x}{t} = \lambda_1 = 0$ are defined below. If $\hat{u}_{LR} - \hat{c}_{LR}$ is positive, we get :

$$Y_{1,l} - Y_L = 0$$

Otherwise, if $\hat{u}_{LR} - \hat{c}_{LR}$ is negative, we get :

$$Y_{3,r} - Y_{3,l} = \beta_3 \hat{r}_3$$

which obviously turns to :

$$Y_{3,r} - Y_L = Y_{1,l} - Y_L = \beta_3 \hat{r}_3$$

We also note that the second component of \hat{r}_3 is null. Hence, we may conclude that in any case:

$$\phi_{1,l} - \phi_L = 0 \quad (2.54)$$

Applying the standard rule (2.52), we also get:

$$\phi_{1,r} - \phi_{1,l} = \beta_1 (\hat{r}_1)_2 = -\beta_1 = -\frac{h}{\hat{u}_{LR}} \quad (2.55)$$

owing to the form of \hat{r}_1 detailed in (2.46).

- If $\hat{u}_{LR} < 0$, we may use a similar construction. Thus, we may conclude that the left and right states of ϕ on each side of the contact discontinuity $\frac{x}{t} = \lambda_1 = 0$ are:

$$\phi_{1,l} = \phi_R + \frac{h}{\hat{u}_{LR}} \quad (2.56)$$

and:

$$\phi_{1,r} = \phi_R \quad (2.57)$$

Obviously , $A(\frac{x}{t} < 0) = A_L$ and $A(\frac{x}{t} > 0) = A_R$. The figure (2.3) shows the different states for the case $\hat{u} > 0$, with $\alpha^+ = \alpha(\phi_{1,r})$ and $\alpha^- = \alpha(\phi_{1,l})$.

In order to go further on, we are compelled to give the explicit form of the source term, so that we may compute the analytic form of $\phi(\alpha)$ through (2.28), which eventually will give α .

We now restrict to the specific choice:

$$s(\alpha) = \frac{\alpha_{eq} - \alpha}{\tau_0}$$

Bound constraints for the void fraction in the linearized Riemann problems:

Both previous interface solvers compute intermediate states which are such that the void fraction α remains within its bounds. If α_L lies in $[0, \alpha_{eq}[$ (respectively α_L lies in $]\alpha_{eq}, 1]$), then for $x/t \in]-\infty, \hat{u}_{LR}[$, we get: $\alpha_L \leq \alpha(x/t) < \alpha_{eq}$ (respectively $\alpha_{eq} < \alpha(x/t) \leq \alpha_L$). In a similar way, if α_R lies in $[0, \alpha_{eq}[$ (respectively α_R lies in $]\alpha_{eq}, 1]$), then for $x/t \in]\hat{u}_{LR}, +\infty[$, we get: $\alpha_R \leq \alpha(x/t) < \alpha_{eq}$ (respectively $\alpha_{eq} < \alpha(x/t) \leq \alpha_R$). \diamond

Proof:

We use previous results and convert relations between $\phi(\alpha)$ states into relations between α states.

– We first suppose $\hat{u}_{LR} > 0$.

Owing to (2.54), if $x/t \in]-\infty, 0[$, we get:

$$\alpha(x/t) = \alpha\left(\frac{x}{t} = 0^-\right) = \alpha_L \quad (2.58)$$

Otherwise we get, using (2.55):

$$\alpha(x/t) = \alpha\left(\frac{x}{t} = 0^+\right) = \alpha_{eq} + e^{-\frac{h}{\tau_0 \hat{u}_{LR}}} (\alpha_L - \alpha_{eq}) \quad (2.59)$$

if $x/t \in]0, \hat{u}_{LR}[$.

The last case leads to :

$$\alpha(x/t) = \alpha_R \quad (2.60)$$

if $x/t \in]\hat{u}_{LR}, +\infty[$.

– On the opposite, if $\hat{u}_{LR} < 0$, we get :

$$\alpha(x/t) = \alpha_L \quad (2.61)$$

if $x/t \in]-\infty, \hat{u}_{LR}[$.

Otherwise, the counterpart of (2.56) provides:

$$\alpha(x/t) = \alpha\left(\frac{x}{t} = 0^-\right) = \alpha_{eq} + e^{\frac{h}{\tau_0 \hat{u}_{LR}}} (\alpha_R - \alpha_{eq}) \quad (2.62)$$

if $x/t \in]\hat{u}_{LR}, 0[$.

The last possibility is :

$$\alpha(x/t) = \alpha\left(\frac{x}{t} = 0^+\right) = \alpha_R \quad (2.63)$$

if $x/t \in]0, +\infty[$, which corresponds to (2.57).

\diamond

Remark 2 (1) *The above property clearly depends on the source term $s(\alpha)$. Bound constraints are also satisfied for a source term of the form $s(\alpha) = \frac{\epsilon}{\tau_0} \alpha(1-\alpha)$, which includes two poles, see appendix 5 in [51] for proof.*

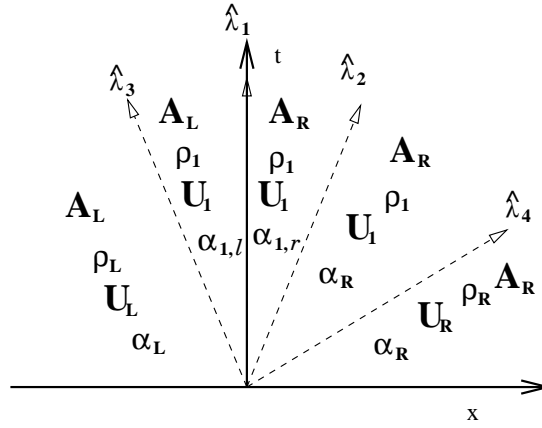


FIG. 2.3 – Sketch of the solution of the one-dimensional linearized Riemann problem when $\hat{\lambda}_2 > 0$.

Remark 3 (2) All computations performed in the next section are based on the use of the first interface Riemann solver with variable $Y(W) = {}^t(A, \phi(\alpha), \rho, u)$. It will be combined with the two cell schemes described in the following section.

Remark 4 (3) Using the variable $V(W) = {}^t(A, I, g(\rho), u)$ with $I = A + u\phi$ seems to be of interest. Actually the Riemann invariants in the 1-field in the linearized system are exactly conserved. However, α is no longer a Riemann invariant in the 3-field, nor in the 4-field. Thus this change of variables has been disregarded since it does not guarantee that the lower and upper bounds of α will be preserved.

2.4.2 Well-balanced schemes

First upwinding scheme S_{UPW1}

For any quantity $D(W(Y))$ chosen among the following: ρ , α , P , u , ϕ , I , or ρu , $\rho u \alpha$, $\rho u^2 + P(\rho)$, we will use the notation:

$$D_{i+1/2}^{*-} = D(W(Y^{Riemann}(x/t = 0^-; Y_i^n, Y_{i+1}^n)))$$

and :

$$D_{i-1/2}^{*+} = D(W(Y^{Riemann}(x/t = 0^+; Y_{i-1}^n, Y_i^n)))$$

The solution $Y^{Riemann}(x/t; Y_L, Y_R)$ stands for the self-similar solution of the Riemann problem associated with (2.45) and initial condition Y_L and Y_R . The asterisk thus means that we focus on the cell interface $x = 0$.

Hence, the approximate Godunov scheme (nicknamed VFRoe-ncv, which has been introduced

in [16], and the basics of which have been recalled above), provides:

$$A_i^{n+1} - A_i^n = 0 \quad (2.64)$$

$$\rho_i^{n+1} - \rho_i^n + \frac{\Delta t}{\Delta x} \left((\rho u)_{i+1/2}^{*-} - (\rho u)_{i-1/2}^{*+} \right) = 0 \quad (2.65)$$

$$(\rho \alpha)_i^{n+1} - (\rho \alpha)_i^n + \frac{\Delta t}{\Delta x} \left((\rho \alpha u)_{i+1/2}^{*-} - (\rho \alpha u)_{i-1/2}^{*+} \right) = 0 \quad (2.66)$$

$$(\rho u)_i^{n+1} - (\rho u)_i^n + \frac{\Delta t}{\Delta x} \left((\rho u^2 + P(\rho))_{i+1/2}^{*-} - (\rho u^2 + P(\rho))_{i-1/2}^{*+} \right) = 0 \quad (2.67)$$

when applied to our system (2.20)-(2.23). The source term $s(\alpha)$ is implicitly contained in the star values, which are given by the interface solver of the previous section. If we take into account (*thanks to our interface solver*) that u and ρ are continuous at $\frac{x}{t} = 0$, and thus that:

$$u_{i\pm 1/2}^{*-} = u_{i\pm 1/2}^{*+} = u_{i\pm 1/2}^* \quad (2.68)$$

and:

$$\rho_{i\pm 1/2}^{*-} = \rho_{i\pm 1/2}^{*+} = \rho_{i\pm 1/2}^* \quad (2.69)$$

this system can be simplified in:

$$A_i^{n+1} - A_i^n = 0 \quad (2.70)$$

$$\rho_i^{n+1} - \rho_i^n + \frac{\Delta t}{\Delta x} \left((\rho u)_{i+1/2}^* - (\rho u)_{i-1/2}^* \right) = 0 \quad (2.71)$$

$$(\rho \alpha)_i^{n+1} - (\rho \alpha)_i^n + \frac{\Delta t}{\Delta x} \left((\rho u)_{i+1/2}^* \alpha_{i+1/2}^{*-} - (\rho u)_{i-1/2}^* \alpha_{i-1/2}^{*+} \right) = 0 \quad (2.72)$$

$$(\rho u)_i^{n+1} - (\rho u)_i^n + \frac{\Delta t}{\Delta x} \left((\rho u^2 + P(\rho))_{i+1/2}^* - (\rho u^2 + P(\rho))_{i-1/2}^* \right) = 0 \quad (2.73)$$

We can notice that the system ((2.71),(2.73)) is conservative.

In the remaining of the paper, this scheme will be referred to as S_{UPW1} .

Second upwinding scheme S_{UPW2}

In section 1, we have seen that $I = (A + u\phi)$ was continuous in the 1-wave, we use this particularity to build a second scheme. Equation on the void fraction α is replaced by the non conservative equation using the variable I :

$$\partial_t (\rho I) + \partial_x (\rho u I) + \phi \partial_x (P) = 0 \quad (2.74)$$

It is easy to verify that this equation is valid for regular solutions. One may also check that jump relations are respected.

The equation (2.74) is discretized, and thus (2.66) is replaced by:

$$(\rho I)_i^{n+1} - (\rho I)_i^n + \frac{\Delta t}{\Delta x} \left((\rho u)_{i+1/2}^{*-} I_{i+1/2}^{*-} - (\rho u)_{i-1/2}^{*+} I_{i-1/2}^{*+} \right) + \frac{\Delta t}{\Delta x} \hat{\phi}_i^n (P_{i+1/2}^{*-} - P_{i-1/2}^{*+}) = 0 \quad (2.75)$$

Since we use the same interface Riemann solver, equations (2.68) and (2.69) still hold. For all i we note:

$$I_{i+1/2}^{*-} = A_i + u_{i+1/2}^* \phi_{i+1/2}^{*-} \quad (2.76)$$

$$I_{i+1/2}^{*+} = A_{i+1} + u_{i+1/2}^* \phi_{i+1/2}^{*+} \quad (2.77)$$

where $\phi_{i+1/2}^{*\pm}$ is directly computed by the interface solver, using $Y(W) = {}^t(A, \phi, \rho, u)$. The equation (2.75) becomes:

$$(\rho I)_i^{n+1} - (\rho I)_i^n + \frac{\Delta t}{\Delta x} \left((\rho u)_{i+1/2}^* I_{i+1/2}^{*-} - (\rho u)_{i-1/2}^* I_{i-1/2}^{*+} \right) + \frac{\Delta t}{\Delta x} \hat{\phi}_i^n (P_{i+1/2}^* - P_{i-1/2}^*) = 0 \quad (2.78)$$

where:

$$\hat{\phi}_i^n = \frac{1}{2} \left(\phi_{i+1/2}^{*-} + \phi_{i-1/2}^{*+} \right) \quad (2.79)$$

The next time step requires the computation of ϕ_i^{n+1} through:

$$(\rho u)_i^{n+1} \phi_i^{n+1} = (\rho I)_i^{n+1} - \rho_i^{n+1} A_i \quad (2.80)$$

In the remaining of the paper, this scheme will be referred to as $SUPW2$.

2.5 Numerical results

We now provide some results which have been obtained using the latter three schemes. The three test cases have exact unsteady solutions including discontinuities. In the following, the fractional step method, the scheme with standard upwinding of source terms, and the modified scheme including upwinding of source terms are nicknamed S_{FS} , S_{UPW1} and S_{UPW2} respectively.

We will use the following equation of state for our computations:

$$P(\rho) = K\rho^2 \quad \text{with: } K = 10^5$$

The source term takes the form: $S(\alpha) = (\alpha_{eq} - \alpha)/\tau_0$, with $\alpha_{eq} = 0.5$. We have used two distinct values for the time scale which are $\tau_0 = \{10^{-4}, 10^{-6}\}$.

2.5.1 Expected rates of convergence

We will use the following notations when computing the L^1 norm of the error $e(\Delta x, T)$ a time $t = T$:

$$e(\Delta x, T) = C(T)(\Delta x)^\beta \tag{2.81}$$

The (measured) constant β will denote the rate of convergence.

Actually, for all test cases, α is governed by :

$$\partial_t(\alpha) + u\partial_x(\alpha) = s(\alpha) \tag{2.82}$$

Formally, if the source term is null $s = 0$, the expected rate of convergence for α (for a so-called first-order scheme) will be $1/2$ (see [31] for instance), since the field $\lambda_2 = u$ corresponds to a *contact discontinuity*. Moreover, if $u\partial_x(\alpha) = 0$, the expected rate of convergence for approximate solutions of (2.82) with help of S_{FS} is 1. Hence, unless $u\partial_x(\alpha) = 0$ everywhere, α varies through the contact discontinuity associated with $\lambda_2 = u$, and the leading error will thus be imposed by the convective part on fine meshes (when Δx tends towards 0). We may thus expect that the global rate of convergence for S_{FS} will be $\beta_{FS} = 1/2$.

If we turn to the schemes S_{UPW1} and S_{UPW2} , the appendix A shows that the source term approximation is also of order 1 with respect to Δt , and thus of order 1 with respect to Δx owing to the CFL constraint:

$$(|u| + c)\Delta t/\Delta x = CFL_0$$

Therefore, we may also expect that both S_{UPW1} and S_{UPW2} asymptotic rates of convergence for approximate solutions of (2.82) will be equal to the lower order imposed by the convective operator, that is $\beta_{UPW1} = \beta_{UPW2} = 1/2$.

This pattern should be retrieved for fine enough meshes for all schemes.

According to appendix A, we may also expect that if the non dimensional coefficient $1 - e^{-\Delta x/(U_0\tau_0)}$ is a poor approximation of $\Delta x/(U_0\tau_0)$, which occurs when Δx is not small enough, the approximation of the source term connected with S_{UPW1} will be worse than the one associated with S_{UPW2} or S_{FS} .

2.5.2 Description of the numerical tests

We will focus here on three Riemann problems which involve:

- (i) a pure contact discontinuity including a jump of the void fraction α ;
- (ii) a standard shock tube with uniform void fraction over space;
- (iii) a standard shock tube with discontinuous initial values of α .

We use circles to represent the discrete solution for the first cell scheme S_{UPW1} , while the stars refer to results obtained with the second cell scheme S_{UPW2} . The coarse and the finer mesh contain 100 and 150000 regular cells respectively. For all test cases, the CFL number is set to $CFL_0 = 0.5$. The figure (2.13) gathers all measured errors for each test case and for the three schemes, when $\tau_0 = 10^{-4}$. The figure (2.14) corresponds to the measure of the L^1 norm of the error for the test case (iii) when using scheme S_{UPW1} and $\tau_0 = 10^{-6}$. All so-called measured rates of convergence have been estimated using the finest two grids.

Pure contact discontinuity including a jump of the void fraction α

The initial condition of the Riemann problem will be the following:

	LEFT	RIGHT
U	10	10
RHO	1	1
ALPHA	1	0.6

This results in an unsteady contact discontinuity which moves to the right at speed $\sigma = 10$. Both the pressure and the velocity remain uniform over time and space: $\rho(x,t) = 1$ and $u(x,t) = 10$.

In this test case, $u\partial_x(\alpha)$ is non zero. Actually, the exact solution for the void fraction is:

$$\begin{cases} \alpha(x,t) = \alpha_l(t), & \text{if } x < \sigma t \\ \alpha(x,t) = \alpha_r(t), & \text{if } x > \sigma t \end{cases}$$

The function $\alpha_l(t)$ (resp. $\alpha_r(t)$) is solution of the ODE: $\partial_t(\alpha) = s(\alpha)$, with initial condition $\alpha(0) = \alpha_L$ (resp. with initial condition $\alpha(0) = \alpha_R$). Of course, both relax to:

$$\alpha_{eq} = 0.5$$

The time scale is $\tau_0 = 10^{-4}$. In figure (2.4), the solution is plotted at time $T_{max} = 3.8729 \cdot 10^{-4}$ when the mesh contains 5000 cells. The final values are $\alpha_l(T_{max}) = 0.51039$ and $\alpha_r(T_{max}) = 0.50208$.

Both the discrete values of velocity and pressure remain constant (thus the error is null). A glance at figure (2.4) clearly shows that the approximate values of the void fraction which have been computed with schemes S_{FS} and S_{UPW2} are almost the same. However, though the scheme S_{UPW1} correctly predicts the position of the contact wave, associated amplitudes of α on both sides are not very accurate on a mesh containing 5000 cells. As shown in appendix A, the local parameter which governs the accuracy on the void fraction, that is: $coef = 1 - e^{-\Delta x/(U_0\tau_0)}$, should be a decent approximation of $\Delta x/(U_0\tau_0)$. It thus clearly appears that in the low Mach number regions, the approximation gets worse, and this is obviously depicted in figure (2.5).

The L^1 norm of the error for the component α can be found on the top of figure (2.13). One may note that the *measured* rate is approximately equal to $\beta_{UPW1} = 0.98$, $\beta_{UPW2} = 0.55$ and

$\beta_{FS} = 0.51$ for schemes S_{UPW1} , S_{UPW2} and S_{FS} respectively. The rates of convergence for the α component are thus identical for S_{UPW2} and S_{FS} . On each side of the contact discontinuity travelling at speed $\sigma = 10$, both discrete values of u and P remain uniform, together with α . Thus, following appendix A, schemes S_{UPW2} and S_{FS} provide the same nice approximation of α , which results in a very similar error level on all mesh sizes, and a similar measured rate of convergence which is very close to the asymptotic rate $1/2$.

The reason why the measured rate of convergence for S_{UPW1} is close to 1, and far from $1/2$, is due to the fact that the mesh size of the finest meshes is still too coarse to observe the asymptotic rate of convergence, which is confirmed by the rather high level of the error.

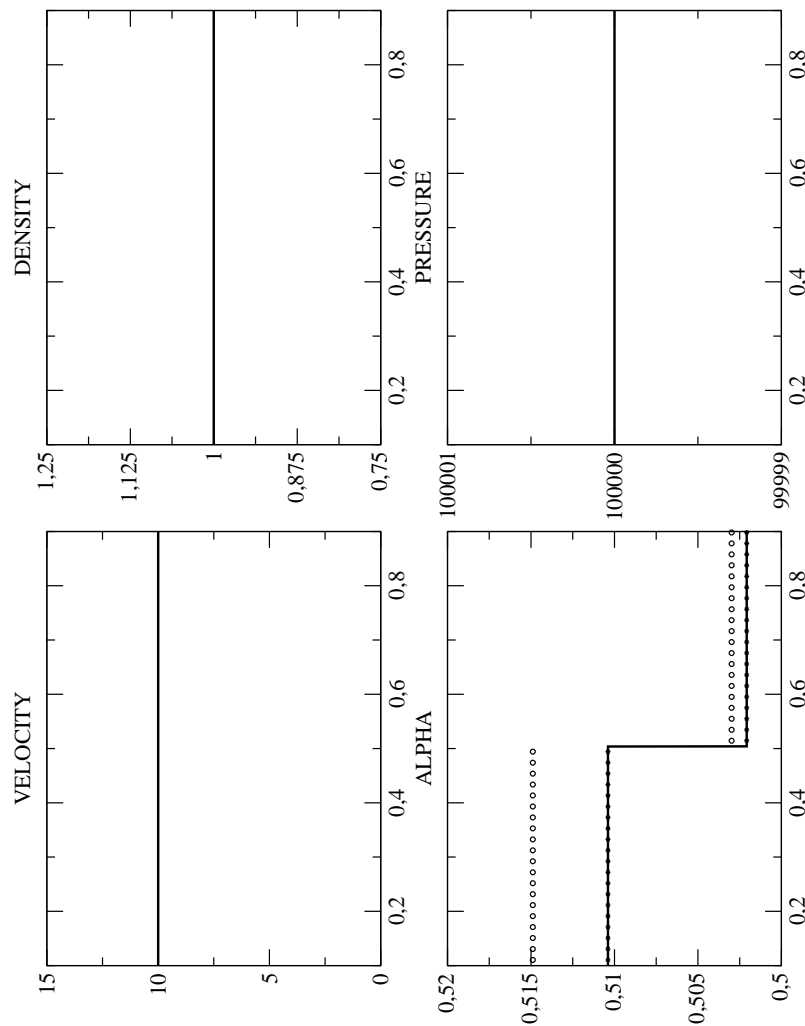


FIG. 2.4 – Numerical solutions for the contact wave (5000 cells) circles S_{UPW1} , black circles S_{UPW2} , continuous line S_{FS}

A standard shock tube with uniform void fraction over space

Initial condition:

	LEFT	RIGHT
U	10	10
RHO	1	0.5
ALPHA	1	1

The density-velocity solution is composed of a 3-rarefaction wave and a 4-shock wave, the 3-wave expands to the left and the 4-wave goes to the right boundary. Once again, the void fraction state is relaxed to α_{eq} by the source term, with a one-state pattern (there is no influence of the genuinely non linear fields on the void fraction profile). The time scale is once more $\tau_0 = 10^{-4}$ and the solution is plotted at time $T_{max} = 3.8729 \cdot 10^{-4}$ when the mesh contains 5000 cells. The final (uniform) value of the void fraction is $\alpha_l(T_{max}) = \alpha_r(T_{max}) = 0.51039$. As in the previous case (see figure (2.5)), the scheme S_{UPW1} provides a rather poor approximation of the solution α , but the error is even more important here, which once more can be easily explained on the basis of Appendix A.

This case is somewhat specific since $u\partial_x(\alpha) = 0$. Thus, the scheme S_{FS} behaves very well, since no error due to the approximation of the convective system arises, which is combined with the fact that S_{FS} exactly integrates source terms within the second step. One should thus keep in mind that this is probably the best set of initial conditions for the latter scheme S_{FS} . Actually, the error for S_{FS} is almost due to round-off errors, and the measured rate of convergence is meaningless.

On the contrary, the *measured* rates of convergence for schemes S_{UPW1} , S_{UPW2} are approximately equal to $\beta_{UPW1} = 1.005$ and $\beta_{UPW2} = 0.997$ respectively. This means that for that range of meshes, the leading error is still due to the approximation of the source term. As expected, the corrected scheme S_{UPW2} nonetheless performs much better than S_{UPW1} , as confirmed by the error analysis (see middle of figure (2.13)). However, the error for α due to S_{UPW2} is rather small on the left side and on the right side of the computational domain, where u , α and ρ remain uniform -which agrees with the analysis of appendix A -, but is no longer small in the intermediate region where gradients of u and ρ develop. One thus retrieves that the leading error within this range of meshes is still due to the approximation of sources even for the best-suited upwinding scheme S_{UPW2} , which implies that the measured rate of convergence for S_{UPW2} is still far from the asymptotic rate 1/2.

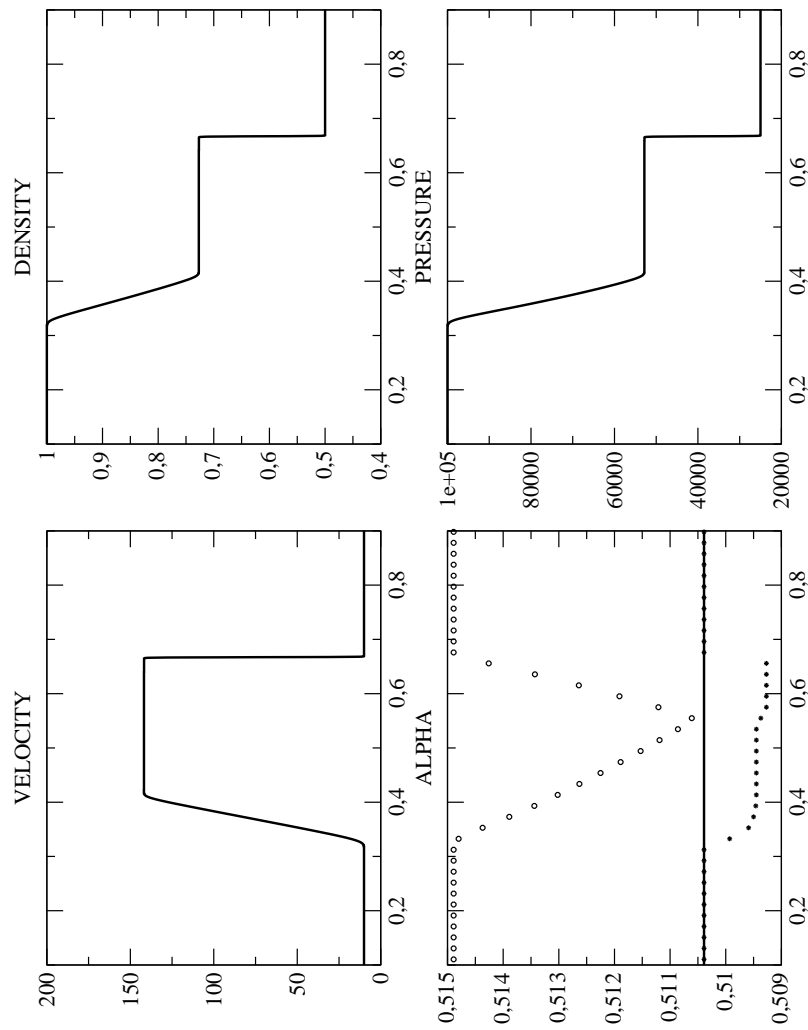


FIG. 2.5 – Numerical solutions for the shock tube test case (5000 cells) circles S_{UPW1} , black circles S_{UPW2} , continuous line S_{FS}

A standard shock tube with discontinuous initial values of α

Initial condition:

	LEFT	RIGHT
U	10	10
RHO	1	0.5
ALPHA	1	0.6

The basic solution on (u, P) is the same as in the previous case, but we no longer have the restriction $u\partial_x(\alpha) = 0$. Once again, the void fraction state is "relaxed" to α_{eq} by the source term, with a two-state pattern as in the first case (there is no influence of the genuinely non linear fields on the void fraction profile). The only difference with the first test case is that the speed of the contact discontinuity is now $u = U_l = U_r$ where the l, r subscripts refer to both sides of the 2-contact discontinuity. Hence, the void fraction discontinuity moves at speed $u \sim 150$. The mesh still contains 5000 cells, the final time is: $T_{max} = 3.8729 \cdot 10^{-4}$, and we also have: $\alpha_l(T_{max}) = 0.51039$ and $\alpha_r(T_{max}) = 0.50208$.

Comments pertaining to the three schemes remain almost the same here (see figure (2.6)). The corrected scheme S_{UPW2} performs better in the low Mach number regions, unlike the basic upwinding technique S_{UPW1} . However, the approximations provided by S_{UPW2} are less accurate in the regions where u and ρ profiles develop, compared with zones where both u and ρ are uniform. The scheme S_{FS} still behaves very well.

More precisely, the *measured* rates of convergence are approximately $\beta_{UPW1} = 0.975$, $\beta_{UPW2} = 0.842$ and $\beta_{FS} = 0.501$ for S_{UPW1} , S_{UPW2} and S_{FS} respectively (see bottom of figure (2.13)). For this test case, error levels for the three schemes are much closer to one another, but the patterns mentioned above remain unchanged. The measured rate of convergence for S_{FS} is close to the asymptotic rate $1/2$, and the measured rate of convergence for S_{UPW1} is still close to 1, though we expect $1/2$.

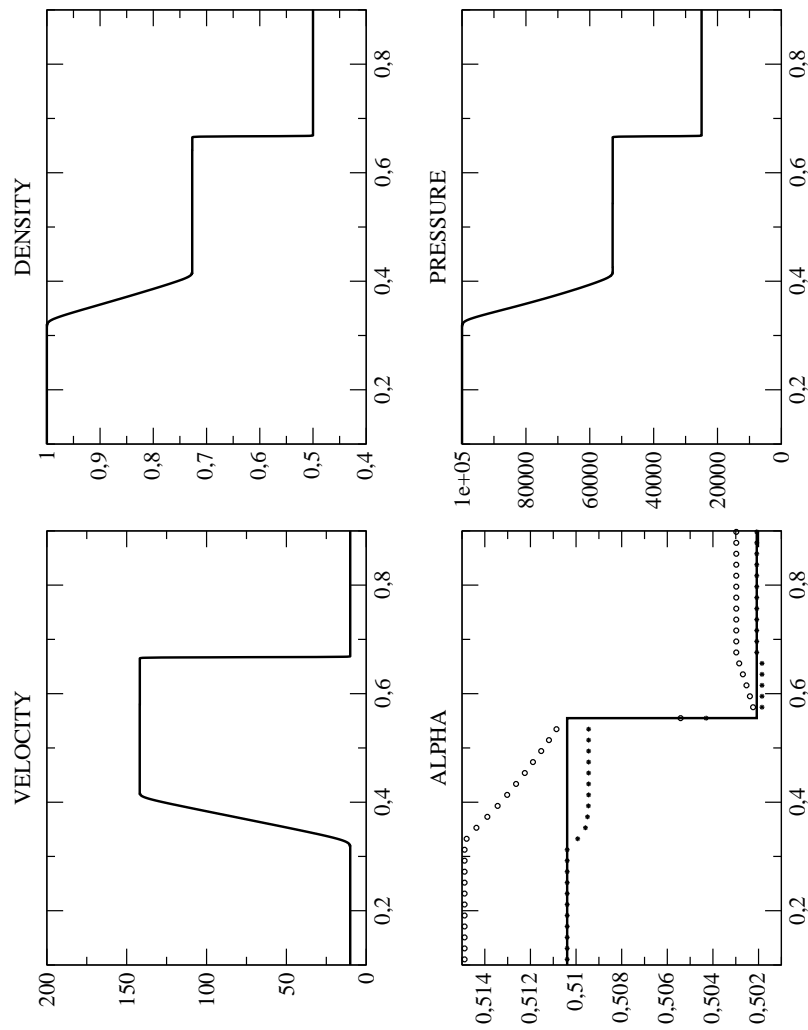


FIG. 2.6 – Numerical solutions for the standard shock tube with α discontinuity circles S_{UPW1} , black circles S_{UPW2} , continuous line S_{FS}

2.5.3 Results on the coarsest mesh ($\tau_0 = 10^{-4}$)

We still consider the same test cases but we now only plot results obtained with a coarse mesh with 100 cells (which corresponds to a very coarse mesh such as those used in the industrial framework). We plot separately the results obtained with S_{FS} , and (S_{UPW1} , S_{UPW2}).

Pure contact discontinuity including a jump of the void fraction α

The initial data has been detailed in section 5.2.1. Results are given in figures (2.7), (2.8). The solution is now plotted at time $T_{max} = 3.940 \cdot 10^{-4}$. The final values are now $\alpha_l(T_{max}) = 0.50976$ and $\alpha_r(T_{max}) = 0.50194$.

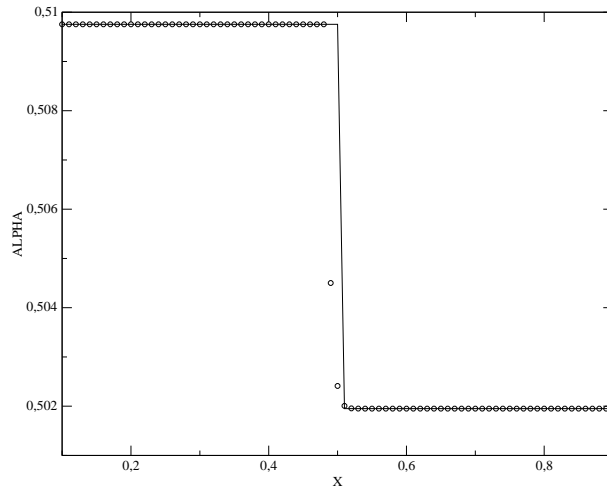


FIG. 2.7 – Fractional step method S_{FS} - 100 cells - Pure contact discontinuity. The continuous line refers to the exact solution. The initial data is given in section 5.2.1. $T_{max} = 3.94 \cdot 10^{-4}$, $\alpha_l(T_{max}) = 0.50976$, $\alpha_r(T_{max}) = 0.50194$

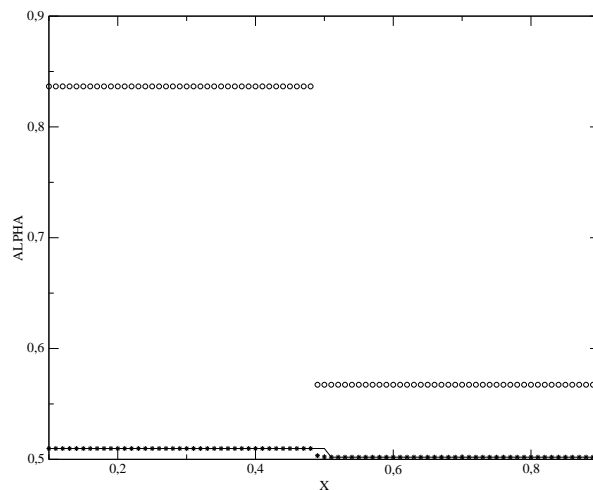


FIG. 2.8 – First and second cell schemes for Leroux method S_{UPW1} , S_{UPW2} - 100 cells - The continuous line refers to the exact solution. The initial data is given in section 5.2.1.

A standard shock tube with uniform void fraction over space

The initial data has been detailed in section 5.2.2. Results are given in figures (2.9), (2.10).

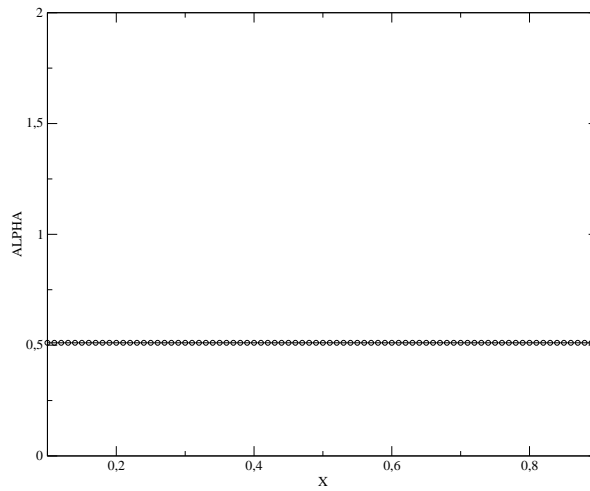


FIG. 2.9 – *Fractional step method S_{FS} - 100 cells - Shock wave with uniform void fraction profile. The initial data is given in section 5.2.2. The continuous line refers to the exact solution. $T_{max} = 3.8729 \cdot 10^{-4}$, $\alpha_l(T_{max}) = 0.51039$, $\alpha_r(T_{max}) = 0.51039$*

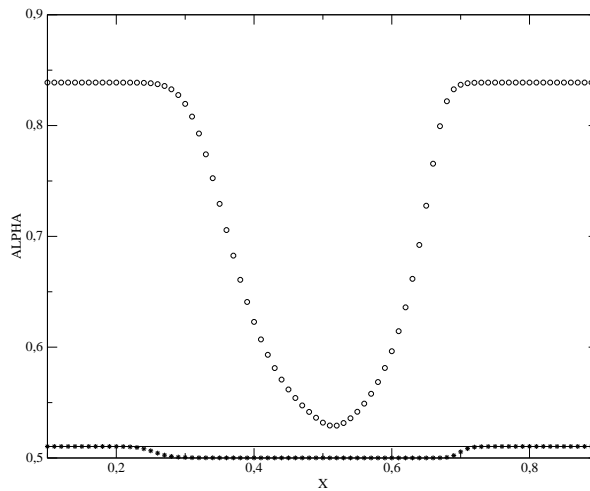


FIG. 2.10 – *First and second cell schemes for Leroux method S_{UPW1} , S_{UPW2} - 100 cells - The continuous line refers to the exact solution. The initial data is given in section 5.2.2.*

A standard shock tube with discontinuous initial values of α

The initial data has been detailed in section 5.2.3. Results are given in figures (2.11), (2.12).

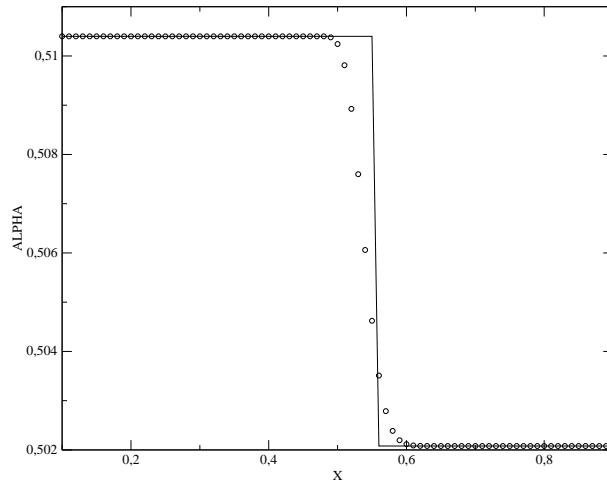


FIG. 2.11 – *Fractional step method S_{FS} - 100 cells - Shock wave including void fraction disequilibrium. The initial data is given in section 5.2.3. The continuous line refers to the exact solution. $T_{max} = 3.8729 \cdot 10^{-4}$, $\alpha_l(T_{max}) = 0.51039$, $\alpha_r(T_{max}) = 0.50208$*

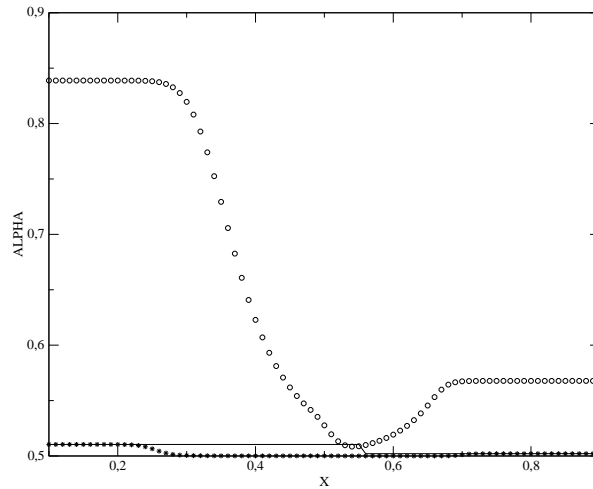


FIG. 2.12 – *First and second cell schemes for Leroux method S_{UPW1} , S_{UPW2} - 100 cells - The continuous line refers to the exact solution. The initial data is given in section 5.2.3.*

Remark 5 (4) *When $\tau_0 = 10^{-6}$, convergence results for the standard shock tube with discontinuous initial values of α (section 5.2.3) show that (see figure (2.14)): (i) the error is negligible when using S_{UPW2} or S_{FS} , (ii) the error for S_{UPW1} (circles) is non negligible on coarse meshes only.*

Remark 6 (5) *Of course, one should keep in mind the fact that rates of convergence would be better when computing approximations of regular solutions.*

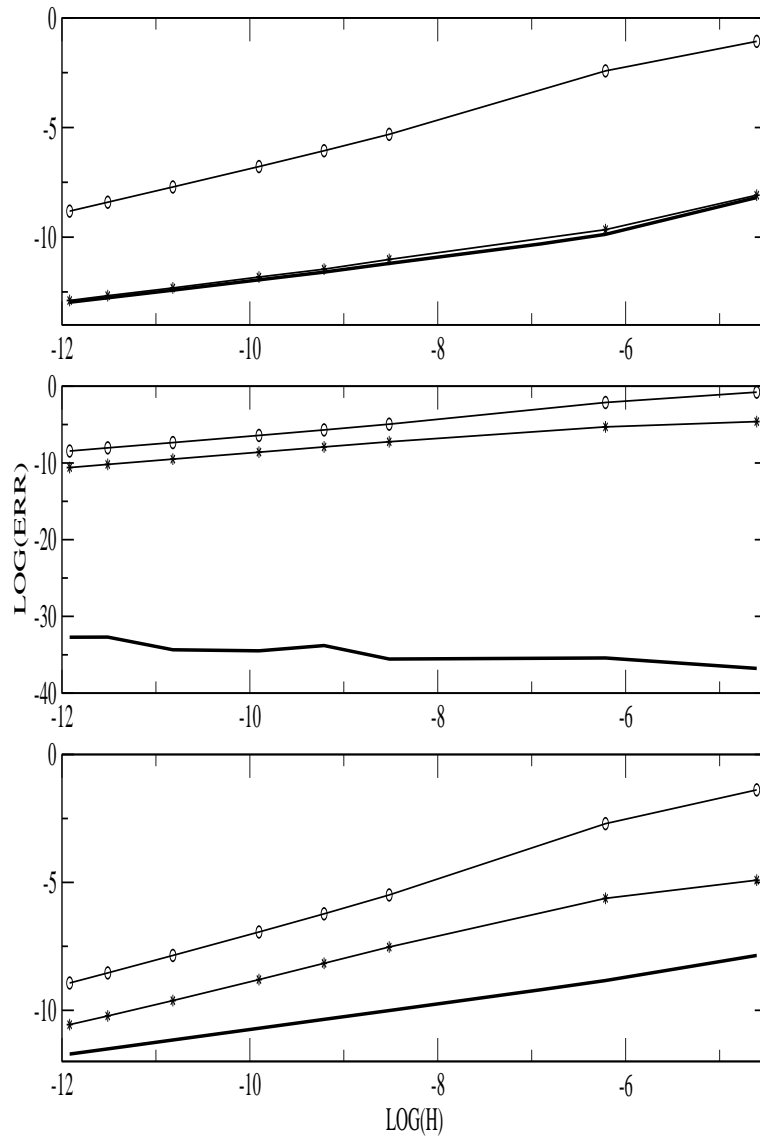


FIG. 2.13 – Convergence in L_1 norm for $\alpha - \tau_0 = 10^{-4}$ - Pure contact discontinuity, see section 5.2.1 (top) Shock wave with uniform void fraction profile, see section 5.2.2 (middle) Shock wave including void fraction disequilibrium, see section 5.2.3 (bottom) Symbols: circles S_{UPW1} , stars S_{UPW2} , continuous line S_{FS}

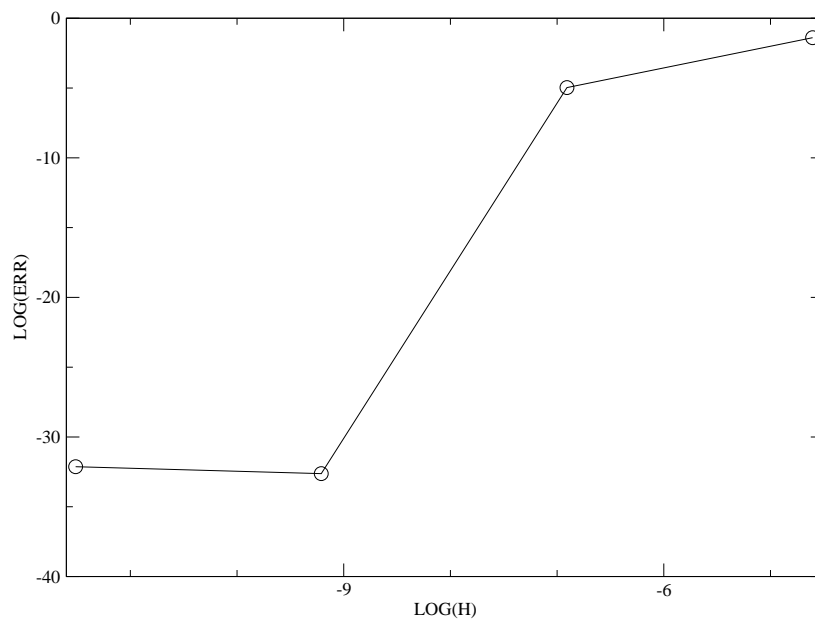


FIG. 2.14 – *Convergence in L_1 norm - $\tau_0 = 10^{-6}$ - Shock wave including void fraction disequilibrium circles S_{UPW1}*

2.6 Concluding remarks

The three schemes converge towards the correct solutions, when focusing on our unsteady tests cases. For all test cases the *measured* rate of convergence for the fractional step method S_{FS} is close to the asymptotic rate $1/2$ (unless meaningless), whereas the *measured* rate of convergence for the basic upwinding technique S_{UPW1} is far from the asymptotic rate $1/2$ and indeed close to 1. The *measured* rate of convergence for the new upwinding approach S_{UPW2} lies in $[1/2,1]$, depending on the test case. For these *unsteady* test cases, the observed performances indicate that the best approximations are provided by S_{FS} , and that those of S_{UPW1} are rather poor, whatever the mesh size is. We must recall here once more that the basic motivation of S_{UPW1} concerns the accurate approximation of *steady* states. The new scheme S_{UPW2} attempts to benefit from advantages of the upwinding approach (devoted to steady cases) and meanwhile it aims at providing better approximations than S_{UPW1} in unsteady cases. Results are in agreement with expectations. However, it is not clear whether one may easily derive the counterpart of S_{UPW2} , for any non-homogeneous hyperbolic system.

More precisely, concerning the effective accuracy of schemes, we also have a fourfold conclusion as follows:

- The two schemes S_{UPW2} and S_{FS} have a similar behavior. The first one S_{UPW2} is the best one for steady computations, the second one is favoured when highly time dependent solutions develop, especially if convective terms are negligible when compared with (stiff) source terms,
- If $\Delta t \ll \tau_0$, S_{FS} performs quite well,
- The scheme S_{UPW1} is of course excellent for *steady* computations,
- If $\frac{\Delta x}{U_0 \tau_0}$ is not small compared with 1, the scheme S_{UPW1} provides rather poor numerical results in highly *unsteady* cases on coarse meshes (though the approximate solution still converges to the exact solution when the mesh size tends to 0) . This is obviously not in favour of: (a) low Mach number areas ; (b) small time scales τ_0 (that is stiff source terms).

Further improvements are necessary in order to deal with the computation of unsteady solutions of hyperbolic systems with source terms. This is particularly urgent for those who wish to tackle with problems such as those arising in the interfacial coupling of thermohydraulic two-phase flow models (see [2], [7], and [52], [53] for instance). These models involve very different time scales in associated source terms. A straightforward dramatic consequence of the occurrence of the stiff source terms is that the accuracy of unsteady computations will diminish when using well-balanced schemes. Actually, it must be noted that the difference of behavior between the fractional step method and the well-balanced scheme is emphasized by this kind of systems. The situation will be different -and the difference between schemes less sensitive- for other non-homogeneous systems such as the shallow water equations with topography, since these involve source terms which directly contribute to the amplitude of the speed of waves (see [33]), but do not contain independent time scales, unless friction terms are accounted for.

Eventually, one should also note that the use of higher order schemes will not qualitatively change the relative behaviour of both schemes, in a similar framework.

Acknowledgments:

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2.7 Appendix A

We want here to highlight the relaxation behavior of the different schemes by using particular initial data.

The source term is chosen as :

$$s(\alpha) = \frac{\alpha_{eq} - \alpha}{\tau_0}$$

We choose the case where $\alpha_L = \alpha_R$ are greater than α_{eq} .

As initial data we choose for all cell i : $u_i^0 = u_0 > 0$ and $P_i^0 = P_0$ or equivalently $\rho_i^0 = \rho_0$.

The equation (2.70) gives $A_i^{n+1} = A_i^n$. Due to the VFRoe-ncv scheme, the equation (2.71) implies that $\rho_i^{n+1} = \rho_i^n$, and the equation (2.73) implies that $u_i^{n+1} = u_i^n$. Thus we have for all cell i and at any time t^n , $u_i^n = u_0$ and $\rho_i^n = \rho_0$.

2.7.1 Well-balanced scheme (S_{UPW1})

The equation (2.72) becomes:

$$\alpha_i^{n+1} - \alpha_i^n + \frac{\Delta t}{\Delta x} u_0 \left(\alpha_{i+1/2}^{*-} - \alpha_{i-1/2}^{*+} \right) = 0$$

Using the Riemann solver of section 3.1 and setting $\beta = e^{-\frac{\Delta x}{\tau_0 u_0}}$, $\lambda = \frac{\Delta t}{\Delta x}$, we have:

$$\alpha_{i+1/2}^{*-} = \alpha_i^n$$

$$\alpha_{i-1/2}^{*+} = \alpha_{i-1}^n \beta + \alpha_{eq} (1 - \beta)$$

and equation (2.66) finally becomes:

$$\alpha_i^{n+1} - \alpha_i^n + \lambda u_0 (\alpha_i^n - \alpha_{i-1}^n) = \lambda u_0 (1 - \beta) (\alpha_{eq} - \alpha_{i-1}^n) \quad (2.83)$$

The assumption on the initial values of α leads us to write $\alpha_i^n = \alpha_{i-1}^n = \alpha^n$. Thus (2.83) reads :

$$\alpha^{n+1} = \alpha^n + \lambda u_0 (1 - \beta) (\alpha_{eq} - \alpha^n) \quad (2.84)$$

The particular initial data allows us to focus on the relaxation behavior of α due to source term. In order to have a good relaxation behavior, the equation (2.84) must provide a consistent approximation of the solution of (2.40),(2.41), or equivalently of: $\partial_t(\alpha) = s(\alpha)$, that is:

$$\alpha(x, t^n + \Delta t) = \alpha(x, t^n) e^{-\frac{\Delta t}{\tau_0}} + \alpha_{eq} (1 - e^{-\frac{\Delta t}{\tau_0}}) \quad (2.85)$$

or at least with the discretized form of (2.40),(2.41), which is:

$$\alpha^{n+1} = \alpha^n + \frac{\Delta t}{\tau_0} (\alpha_{eq} - \alpha^n) \quad (2.86)$$

In order to have a similar behavior the relation $\frac{\Delta t}{\tau_0} \sim \lambda u_0 (1 - \beta)$ has to hold. This relation leads to $\frac{\Delta x}{\tau_0 u_0} \sim 0$. Obviously, it will not be satisfied on coarse meshes, especially when either the time scale, or the local velocity is small.

2.7.2 Well-balanced scheme (S_{UPW2})

Inserting the initial data in (2.75) leads to:

$$I_i^{n+1} - I_i^n + \lambda u_0 (I_i^n - I_{i-1}^n) = 0 \quad (2.87)$$

which can be written:

$$\phi(\alpha_i^{n+1}) - \phi(\alpha_i^n) + \lambda(\Delta x + u_0\phi(\alpha_i^n) - u_0\phi(\alpha_{i-1}^n)) = 0 \quad (2.88)$$

Thanks to the initial data $\alpha_i^n = \alpha_{i-1}^n = \alpha^n$, we get:

$$\alpha^{n+1} = (\alpha^n - \alpha_{eq})e^{-\frac{\Delta t}{\tau_0}} + \alpha_{eq} \quad (2.89)$$

So that to have the same behavior than (2.86) we must have $\Delta t \ll \tau_0$.

2.7.3 Fractional step scheme (S_{FS})

In the fractional step method, α^{n+1} is build up in two steps. First, the Riemann solver computes the convective part of the system; thus, owing to the specific initial data, the convective step is a ghost step for α . The second step is the relaxation due to the source term which is here :

$$\partial_t(\alpha) = s(\alpha) = \frac{\alpha_{eq} - \alpha}{\tau_0} \quad (2.90)$$

Thanks to the form of $s(\alpha)$ we can exactly integrate (2.90) :

$$\alpha^{n+1} = (\alpha^n - \alpha_{eq})e^{-\frac{\Delta t}{\tau_0}} + \alpha_{eq} \quad (2.91)$$

Note that (2.91) is the same equation than for the scheme S_{UPW2} . This explains why approximations of α by S_{UPW2} and S_{FS} are the same in regions where α , ρ and u profiles are uniform.

Hence in order to obtain the same behavior than (2.86) we must have $\Delta t \ll \tau_0$.

Chapitre 3

Couplage interfacial des modèles des équations d'Euler en configuration isentropique à une et deux dimensions d'espace

Le circuit primaire d'une centrale nucléaire est principalement constitué de la cuve, d'une pompe et de tuyaux. Il s'agit d'un circuit fermé d'eau pressurisée dont la circulation est maintenue par la pompe. L'eau est chauffée en passant entre les barreaux de combustible du coeur, dans la cuve, elle est ensuite acheminée par la tuyauterie vers le générateur de vapeur puis retourne, via la tuyauterie, dans la cuve pour recommencer un cycle. Le générateur de vapeur est un échangeur thermique avec le circuit secondaire (fermé lui aussi), et sert à produire de la vapeur d'eau dans ce dernier. Cette vapeur servira à entraîner les turbines génératrices de courant.

Nous nous intéressons dans ce chapitre à la manière de raccorder les tuyaux à la cuve. Etant donnée la petite section des tubes utilisés devant leur longueur, les codes de calcul simulant les écoulements dans ces parties du primaire sont basés sur des modèles mono-dimensionnels. A l'inverse, dans la cuve, la simulation des écoulements fait appel à des modèles tri-dimensionnels. C'est sur cette différence structurelle entre les modèles que nous allons nous focaliser. Pour cela nous supposerons que les modèles thermodynamiques de la cuve et des tubes sont identiques à l'exception de la dimension d'espace. De plus, afin de pallier au temps de calcul exorbitant du 3D et afin de fournir des résultats de convergence significatifs, nous admettrons que la cuve est modélisée en deux dimensions d'espace.

Nous nous proposons donc de coupler le modèle des équations d'Euler isentropique à une dimension d'espace (tube) et le modèle des équations d'Euler isentropique à deux dimensions d'espace (cuve). Les méthodes proposées ne sont pas restrictives et des modèles comprenant notamment une équation d'énergie totale sont brièvement présentés en annexe. Les systèmes sont donc, pour les tubes:

$$\begin{cases} \partial_t (W_1) + \partial_x (F(W_1)) = 0 \\ W_1 = (\rho, \rho u) \\ F(W_1) = (\rho u, \rho u^2 + P(\rho)) \end{cases}$$

et pour la cuve:

$$\begin{cases} \partial_t (W_2) + \partial_x (G_1(W_2)) + \partial_y (G_2(W_2)) = 0 \\ W_2 = (\rho, \rho u, \rho v) \\ G_1(W_2) = (\rho u, \rho u^2 + P(\rho), \rho uv) \\ G_2(W_2) = (\rho v, \rho uv, \rho v^2 + P(\rho)) \end{cases}$$

où ρ désigne la densité, P la pression, u la vitesse selon l'axe x et v la vitesse selon l'axe y . La loi d'état de type "stiffened gas" $P(\rho) = P_0 \rho^\gamma - P_\infty$ permettra aussi bien de réaliser des simulations en gaz parfait ($P_\infty = 0$) que de simuler des fluides ayant un comportement proche de celui de l'eau. Sans perte de généralité nous choisirons une interface de couplage verticale, les deux systèmes à coupler s'écrivent donc respectivement pour le tube et la cuve:

$$\begin{cases} \partial_t (\rho) + \partial_x (\rho u) = 0 \\ \partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \\ v(x, t) = 0 \end{cases} \quad \begin{cases} \partial_t (\rho) + \partial_x (\rho u) = 0 \\ \partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \\ \partial_t (\rho v) + \partial_x (\rho uv) = 0 \end{cases} \quad (3.1)$$

Nous utilisons la méthode de couplage par flux suggérée notamment par A.Y. Leroux (voir par exemple [44] et [74]). Il s'agit de construire un modèle d'interface qui permettra, grâce à la résolution d'un problème de Riemann, de calculer les flux qui seront transmis comme conditions aux limites aux codes de part et d'autre de l'interface de couplage. Cette méthode requiert l'introduction d'une variable z qui ne dépend pas du temps et qui prend la valeur 0 dans le domaine mono-dimensionnel et la valeur 1 dans le domaine bi-dimensionnel. Afin de respecter le caractère mono-dimensionnel de l'écoulement dans les tubes, il apparaît que les modèles d'interface doivent respecter une condition d'admissibilité. Celle-ci traduit le fait que lorsque l'on utilise un code 2D sur un maillage composé d'une rangée de mailles 2D pour simuler un système 1D (par exemple: un écoulement dans un tube), le flux sur la composante transverse du moment doit être nulle pour ne pas "faire vivre" la composante transverse de la vitesse. Les modèles respectant cette condition sont dits admissibles. Deux stratégies se sont naturellement dégagées. La première est basée sur un modèle d'interface non conservatif pour la variable v ; tandis que la deuxième utilise un modèle d'interface conservatif. Le flux analytique du modèle d'interface conservatif admissible est une pondération par z des flux des modèles 1D et 2D dont les systèmes d'équations sont (3.1). En ce qui concerne le modèle d'interface non-conservatif admissible, sa jacobienne est une pondération des jacobienes des modèles 1D et 2D.

Des tests numériques ont été réalisés afin de mettre en valeur l'influence des paramètres suivant:

- l'effet du raffinement du maillage;
- l'effet des coefficients de la loi d'état (comportement en eau ou en gaz);
- le positionnement de l'interface par rapport à la jonction entre le tube et la cuve;
- la nature du modèle (conservatif ou non-conservatif).

Les résultats qualitatifs de ces tests tendent à montrer que l'approche non-conservative est nettement préférable à l'approche conservative. En effet les simulations effectuées avec cette dernière montrent un pic de vitesse transverse au niveau de l'interface de couplage, ce qui est préjudiciable surtout si l'on considère une équation de transport pour une espèce chimique. Cette sur-vitesse peut même devenir problématique si l'on considère le système des équations complètes d'Euler (voir annexe), car elle est à l'origine de l'amplification d'un phénomène d'arrière-corps qui conduit à l'apparition du vide. Les résultats confirment aussi qu'en pratique il vaut mieux placer l'interface de couplage suffisamment loin à l'intérieur du tube. Dans cette configuration les fronts d'onde impactant l'interface de couplage sont d'amplitude moindre et les erreurs dues au couplage sont atténuées.

Coupling two and one dimensional unsteady Euler equations through a thin interface

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Abstract : We present herein a method for the numerical coupling of one and two-dimensional Euler isentropic models through a thin interface. The basic approach is connected with recent works by E. Godlewski, A.Y. Leroux and P.A. Raviart. It requires introducing an interface model, and solving the associated Riemann problem at the interface between codes. Numerical results confirm both the stability and the fair accuracy of the admissible non-conservative approach, which is also compared with an admissible conservative approach and a reference two-dimensional solution. The extension to the full Euler set of equations is also briefly discussed.

3.1 Introduction

The problem of the coupling of distinct models described by sets of PDE is a topic which has become of growing interest over the past few years. Actually, it may first occur in the framework of the modelling of two-phase flow in porous media. In that case, one has to face conservation laws with discontinuous flux functions, and one of the main difficulties consists in proving the existence and uniqueness of a physically relevant solution. One may for instance refer to [10], [11], [74] and references therein. It also naturally arises when focusing on industrial projects where computational facilities require the use of different models in order to describe parts of a whole concept. This happens for instance when one aims at computing the flow around a whole plane, or alternatively the flow in a gas turbine engine (decomposed in combustion chamber and turbine section, see [72], [70], [71] for instance). It also immediately occurs when turning to the predictive computations of the flow in the primary coolant circuit of a pressurized water reactor, in a nuclear power plant (see [28]). In the latter case, one sometimes needs to account for the flow in the reactor, in pipes and in the steam generator. Actually, one may apply for a 1D code to deal with the pipe, and a 3D code to predict the flow in the reactor. In addition, the 1D code may include schemes

which provide approximations of a six-equation two-fluid model, whereas the 3D code deals with an homogeneous two phase flow model such as HEM (homogeneous equilibrium model) or HRM (homogeneous relaxation model). The problem of the coupling in such a situation is obviously a tedious and ambitious topic, and it also suggests as a prerequisite that one knows how to couple simpler situations such as the following for instance :

- (i) the coupling of two distinct models in a one dimensional framework ;
- (ii) the coupling of the homogeneous equilibrium model in a 1D pipe and a three dimensional medium.

We will focus in this paper on the problem (ii). We refer for instance to [6], [3], and [55], which try to address the first problem (i) while focusing on HEM and HRM models, and also mention [4], [8] that tackle the coupling of Euler equations with distinct equations of state in each code. We insist that we only want to provide suitable information to be exchanged through the interface, and a (of course stable) numerical way to implement it. Both codes on each side should not be modified by the new procedure, except that boundary conditions may be different from what they were before coupling.

Quite recently, a few authors have suggested some new ideas to couple subsets of PDE. A first approach has been suggested by A.Y. Leroux and co-authors (see [44] for instance). It has been essentially applied to cope with the shallow water equations with topography. The main idea in the latter approach is to include a stationary constraint in the set of PDE with an augmented state variable, and then to solve the exact Riemann problem at the "stationary" interface. The resulting scheme has been proved to be an efficient way to cope with steady state situations ([33]). We emphasize that we will apply for similar ideas in our approach. A second way to tackle with this problem has emerged recently too, and is detailed in [38], [39] in a specific situation. In fact, it may be seen as an extension of ideas in the paper [1], which is roughly grounded on the following idea: initial conditions are used twice to compute two different fluxes at the interface between cells; the first one is obtained solving the exact Riemann problem with the *left* set of PDE, whereas the second one corresponds to the *right* set of PDE. We refer for instance to [6] for more details.

The present paper is organized as follows. We first briefly recall in section 2 the basic sets of equations on each side of the interface between codes. In the beginning of section 3, we exhibit a natural constraint which obviously arises. We then detail a natural interface model and two distinct interface models which may be used to exchange information through the interface for unsteady predictions. The associated left and right fluxes will be detailed. Section 4 is devoted to the presentation of schemes that will be used, and of numerical results. Computational results involving shock waves with great inhomogeneities of transverse velocities between both medium will be discussed, and this will be achieved on the basis of the L^1 norm of the error. Actually, results obtained when computing unsteady solutions traveling from a 2D tank to the 1D pipe will be compared with those obtained while using the 2D code over the whole domain. The comparison will include :

- (a) the effect of mesh refinement;
- (b) the sensitivity with respect to the EOS;
- (c) the influence of the location of the interface between codes on numerical results;
- (d) the influence of the interface model.

For further details, the reader is referred to [55]. The extension of these ideas to the framework of non-isentropic Euler equations is also briefly examined in an appendix.

This work is a contribution to the NEPTUNE joint project, and is part of recent investigations which aim at improving the numerical interfacial coupling of two-phase flow codes (see [49], [51], [55] among others).

3.2 Models

3.2.1 Codes to be coupled

For the sake of simplicity we consider the isentropic Euler model. We want to couple the one-dimensional isentropic Euler system to the two-dimensional isentropic Euler system through a thin interface. Without loss of generality we consider that the interface is along the y -axis.

On the left side of the interface we consider the one-dimensional isentropic Euler system (1D):

$$\partial_t (W_1) + \partial_x (F(W_1)) = 0 \quad (3.2)$$

with:

$$\begin{cases} W_1 = (\rho, \rho u) \\ F(W_1) = (\rho u, \rho u^2 + P(\rho)) \end{cases}$$

where u , ρ and P respectively stand for the velocity, the density and the pressure, with $P'(\rho) > 0$. These variables only depend on the time t and the space dimension x , $W_1 = W_1(x, t)$.

On the right side of the interface we consider the two-dimensional isentropic Euler system (2D):

$$\partial_t (W_2) + \partial_x (G_1(W_2)) + \partial_y (G_2(W_2)) = 0 \quad (3.3)$$

with:

$$\begin{cases} W_2 = (\rho, \rho u, \rho v) \\ G_1(W_2) = (\rho u, \rho u^2 + P(\rho), \rho uv) \\ G_2(W_2) = (\rho v, \rho uv, \rho v^2 + P(\rho)) \end{cases}$$

Here u denotes the component of the velocity along the x -axis and v the component of the velocity along the y -axis. Here all the variables depend on time t and on two space variables x and y , $W_2 = W_2(x, y, t)$.

3.2.2 The one-dimensional model

We recall herein some well-known properties of the conservative system (3.2). This will be useful in section 4.

Eigenstructure

In terms of the variable $Y = (\rho, u)$, and setting $c^2 = P'(\rho)$, (3.2) writes in non-conservative form:

$$\partial_t (Y) + A(Y) \partial_x (Y) = 0$$

where the 2×2 convection matrix A is:

$$A(Y) = \begin{pmatrix} u & \rho \\ \frac{c^2}{\rho} & u \end{pmatrix}$$

The eigenvalues and the right eigenvectors of the matrix A are:

$$\lambda_1 = u - c, \quad r_1^\top = (\rho, -c)$$

$$\lambda_2 = u + c, \quad r_2^\top = (\rho, c)$$

Thus, until vacuum occurs, eigenvalues are real and distinct; the system is unconditionally hyperbolic since the two eigenvectors span the plane \mathbb{R}^2 . Moreover both fields are genuinely non-linear.

Entropy pair

One may easily check that an entropy pair $(\eta(W_1), F_\eta(W_1))$ is:

$$\begin{aligned}\eta(W_1) &= \frac{\rho u^2}{2} + \rho\psi(\rho) \\ F_\eta(W_1) &= (\eta(W_1) + P(\rho))u\end{aligned}$$

with $\psi(\rho) = \int_0^\rho \frac{P(a)}{a^2} da$. Moreover η is strictly convex with respect to W_1 . Hence the Riemann problem associated with (3.2) has a unique entropy consistent solution composed of constant states separated by shocks and rarefaction waves, with no vacuum occurrence, provided that the initial data agrees with the condition:

$$u_R - u_L < g(\rho_L) + g(\rho_R)$$

where: $g'(\rho) = \frac{c(\rho)}{\rho}$ -see [75] and [37] -.

Solution for the Riemann problem

We describe herein the main features of the solution of the Riemann problem.

We set (u_L, ρ_L) and (u_R, ρ_R) the left and right state for the Riemann problem associated with system (3.2). The right and left pressure for initial state are respectively $P_R = P(\rho_R)$ and $P_L = P(\rho_L)$. We set (u^*, ρ^*) to be the intermediate state between the two waves and we set $P^* = P(\rho^*)$.

– Trough the 1-wave, we get:

$$u^* - u_L = h_L(P_L, P^*)$$

If $P_L < P^*$, the 1-wave is a shock wave:

$$h_L(P_L, P^*) = -\sqrt{\frac{(P^* - P_L)(\rho^* - \rho_L)}{\rho_L \rho^*}}$$

otherwise the 1-wave is a rarefaction wave:

$$h_L(P_L, P^*) = g(\rho_L) - g(\rho^*)$$

– Trough the 2-wave, we get:

$$u^* - u_R = h_R(P_R, P^*)$$

If $P_R < P^*$, the 2-wave is a shock wave:

$$h_R(P_R, P^*) = \sqrt{\frac{(P^* - P_R)(\rho^* - \rho_R)}{\rho_R \rho^*}}$$

otherwise the 2-wave this is a rarefaction wave:

$$h_R(P_R, P^*) = g(\rho^*) - g(\rho_R)$$

3.2.3 The two-dimensional model

We can write the system (3.3) in a non-conservative form using the variable $Z^\top = (\rho, u, v)$:

$$\partial_t(Z) + B_x(Z)\partial_x(Z) + B_y(Z)\partial_y(Z) = 0$$

with the following 3×3 matrix B_x and B_y :

$$B_x(Z) = \begin{pmatrix} u & \rho & 0 \\ \frac{c^2}{\rho} & u & 0 \\ 0 & 0 & u \end{pmatrix}$$

$$B_y(Z) = \begin{pmatrix} v & 0 & \rho \\ 0 & v & 0 \\ \frac{c^2}{\rho} & 0 & v \end{pmatrix}$$

For any $(w_1, w_2) \in \mathbb{R}^2 - \{(0,0)\}$ with $w_1^2 + w_2^2 = 1$, we set $C(Z, w) = w_1 B_x(Z) + w_2 B_y(Z)$. The system (3.3) is hyperbolic if for any (w_1, w_2) and for any $Z \in \Omega$, the matrix $C(Z, w)$ has three real eigenvalues and three independent eigenvectors. It is easy to verify that the eigenvalues of $C(Z, w)$ are real:

$$\lambda_1 = (w_1 u + w_2 v)$$

$$\lambda_2 = (w_1 u + w_2 v) - c\sqrt{w_1^2 + w_2^2}$$

$$\lambda_3 = (w_1 u + w_2 v) + c\sqrt{w_1^2 + w_2^2}$$

The corresponding eigenvectors are clearly independent until vacuum occurs:

$$r_1^\top = (0, w_2, w_1)$$

$$r_2^\top = \left(\rho, \frac{w_1 c}{\sqrt{w_1^2 + w_2^2}}, \frac{w_2 c}{\sqrt{w_1^2 + w_2^2}} \right)$$

$$r_3^\top = \left(\rho, -\frac{w_1 c}{\sqrt{w_1^2 + w_2^2}}, -\frac{w_2 c}{\sqrt{w_1^2 + w_2^2}} \right)$$

3.3 The interface model

Obviously, a two-dimensional code (based on a two-dimensional system) applied on a "one-dimensional" domain does not behave as a one-dimensional code (based on a one-dimensional system) on the same domain. Nonetheless we want to look for a condition for a 2D code to behave as a 1D code.

3.3.1 A necessary condition: NSC

Let us first define a test problem resumed on the figure (3.1). A pipe ($x < 0$) is connected to a tank ($x > 0$) at $x = 0$ (see figure (3.1)). Suppose that the domain ($x < 0$) is discretized by a row of rectangular cells with volume $\Delta x \times h$. We note ϕ^{God} the value of the field ϕ given by a Godunov method and the subscripts H_i , B_i , D_i and G_i denote respectively the upper, lower, right and left side of the cell i .

Focusing on the transverse component of the momentum, ρv , we write a Godunov [40] scheme in the domain $x < 0$ as:

$$\begin{aligned} & h\Delta x((\rho v)_i^{n+1} - (\rho v)_i^n) \\ & + \Delta t \Delta x [(\rho v^2 + P)_{H_i}^{God} - (\rho v^2 + P)_{B_i}^{God}] \\ & + h\Delta t [(\rho uv)_{D_i}^{God} - (\rho uv)_{G_i}^{God}] = 0 \end{aligned} \quad (3.4)$$

Let us set, for all cells in the domain $x < 0$, $v_i^n = 0$. Using wall condition [16] as a boundary condition, defining $\overrightarrow{N_{H_i}}$ ($\overrightarrow{N_{B_i}}$ respectively) as the unit outward normal vector on the top wall (bottom wall respectively), the pressure on the boundary of the left domain writes:

$$P_{H_i}^{God} = P^{God}(W_i^n, \hat{W}_{H_i}^n, \overrightarrow{N_{H_i}})$$

$$P_{B_i}^{God} = P^{God}(W_i^n, \hat{W}_{B_i}^n, \overrightarrow{N_{B_i}})$$

where $\hat{W}_{H_i}^n = \hat{W}_{B_i}^n = \hat{W}_i^n = (\rho_i^n, (\rho u)_i^n, -(\rho v)_i^n)$ stands for the mirror state of W_i^n .

Then the above initial condition on the velocity implies that for all cells in the domain $x < 0$:

$$\begin{aligned} P_{H_i}^{God} &= P_i^n = P_{B_i}^{God} \\ v_{H_i}^{God} &= v_{B_i}^{God} = v_{G_i}^{God} = 0 \end{aligned}$$

and if we are in the domain $x < -\Delta x$

$$v_{D_i}^{God} = 0$$

So that if we assume that vacuum does not appear ($\rho_i^n > 0$) in these cells, the preceding equation (3.4) provides $v_i^{n+1} = 0$ for all cells except for the cell i_0 (see figure (3.1)) which has its right side on the interface $x = 0$. Indeed nothing ensures that $v_{D_{i_0}}^{God} = 0$ for this particular cell.

This gives us a necessary and sufficient condition (NSC) for a scheme to fit to pure one-dimensional simulation in the left domain.

Definition:

We will say that the coupling boundary conditions will be admissible if the ρv component of the flux at the interface $x = 0^-$ is null, that means:

$$(NSC) : (\rho uv)^- = 0$$

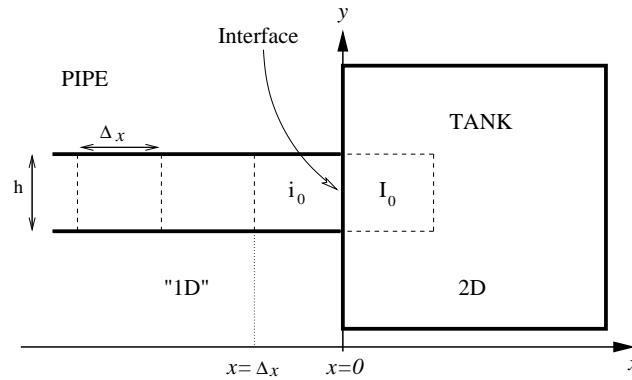


FIG. 3.1 – *The test problem*

We now investigate some possible interface models to couple the one-dimensional domain $x < 0$ to the two-dimensional domain $x > 0$. Interface models are introduced to allow the computation of Godunov fluxes through the vertical interface $x = 0^\pm$. In practice, we recall that they are only used to compute $(\rho uv)(x/t = 0^-)$ and $(\rho uv)(x/t = 0^+)$, as sketched in figure (3.2).

In the left domain we consider the system (3.2) extended with the variable v and one aim of an admissible interface model is to maintain $v = 0$ in this domain by fulfilling the (NSC). An admissible interface model must also give the model (3.2) on the left of the interface and the projection on the normal of the model (3.3) on the right.

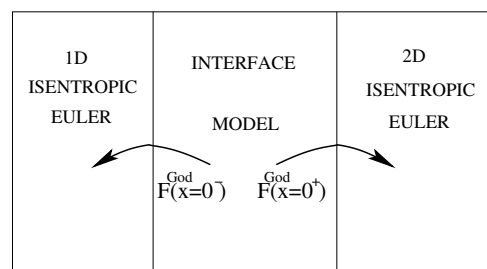


FIG. 3.2 – *The interface model*

We successively consider :

- A natural model at the interface
- A non conservative admissible interface model
- A conservative admissible interface model

3.3.2 A natural model at the interface

An *a priori* obvious candidate as an interface model immediately arises considering the projection on a vertical interface of the model (3.3):

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (3.5)$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (3.6)$$

$$\partial_t (\rho v) + \partial_x (\rho uv) = 0 \quad (3.7)$$

We briefly recall now the structure of the Riemann problem associated with ((3.5)-(3.7)) at the interface $x = 0$ with left state,

$$W_2^L = (\rho_L, \rho_L u_L, \rho_L v_L = 0)^\top$$

and right state,

$$W_2^R = (\rho_R, \rho_R u_R, \rho_R v_R)^\top$$

to determine the Godunov flux at $x = 0^\pm$.

In terms of the variable $Y = (\rho, u, v)^\top$, the eigenvalues and the right eigenvectors of the system (3.5)-(3.7) are:

$$\lambda_1 = u - c, \quad r_1^\top = (\rho, -c, 0)$$

$$\lambda_2 = u, \quad r_2^\top = (0, 0, 1)$$

$$\lambda_3 = u + c, \quad r_3^\top = (\rho, c, 0)$$

The subsystem ((3.5),(3.6)) has been briefly described above. We set u^* and ρ^* the intermediate states for u and ρ between the two waves λ_1 and λ_3 as described below for the system (3.2). We set v_1^* (respectively v_2^*) the intermediate state for v between λ_1 and λ_2 (respectively between λ_2 and λ_3) (see figure (3.3))

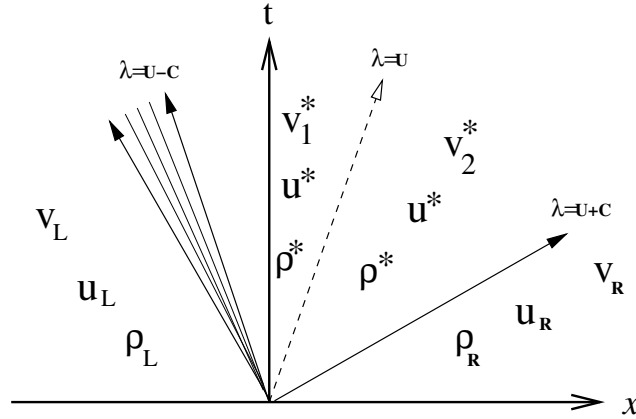


FIG. 3.3 – Intermediate states for u , ρ and v

Focusing on the variable v , we observe that through the first and third waves $[v] = 0$ and that v is a Riemann invariant of the first and third field. Hence the solution for v is, $v_1^* = v_L$ and $v_2^* = v_R$, and so:

$$v(x/t; W_2^L, W_2^R) = \begin{cases} v_L = 0, & \text{if } x/t < u^* \\ v_R, & \text{if } x/t > u^* \end{cases}$$

We assume from now that the 2-wave does not coincide with $x/t = 0$. As a consequence the ρv -component of the Godunov flux at $x/t = 0$ is:

$$(\rho v)(x/t = 0; W_2^L, W_2^R) = \begin{cases} (\rho u)(x/t = 0)v_L = 0, & \text{if } u^* > 0 \\ (\rho u)(x/t = 0)v_R, & \text{if } u^* < 0 \end{cases}$$

Of course, in general $v_R \neq 0$, so that $F^{God}(x = 0^-)$ is not always null if $u^* < 0$. Thus this interface model does not respect the (NSC), which results in the fact that v will not remain zero in the one-dimensional domain.

It must thus be rejected if one aims at computing the solutions in the 1D computational domain with a 2D algorithm and a row of cells.

3.3.3 A non conservative admissible interface model

Following [44] we introduce here a new variable which distinguishes the two domains and does not depend on time t ,

$$z(x, y, t) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases}$$

We now consider the following interface model:

$$\partial_t(z) = 0 \tag{3.8}$$

$$\partial_t(\rho) + \partial_x(\rho u) = 0 \tag{3.9}$$

$$\partial_t(\rho u) + \partial_x(\rho u^2 + P) = 0 \tag{3.10}$$

$$\partial_t(v) + zu\partial_x(v) = 0 \tag{3.11}$$

with initial condition $v(x, y, t = 0) = 0$ for all $x < 0$. We note that (3.11) enables to retrieve

$$\partial_t(v) = 0$$

on the left hand side and

$$\partial_t(v) + u\partial_x(v) = 0$$

on the right hand side -which (thanks to (3.9)), is equivalent to (3.7)-.

Using the set of variables $Y^\top = (z, \rho, u, v)$ the eigenvalues and the right eigenvectors of the system (3.8)-(3.11) are:

$$\lambda_1 = 0, \quad r_1^\top = (1, 0, 0, 0)$$

$$\lambda_2 = u - c, \quad r_2^\top = (0, \rho, -c, 0)$$

$$\lambda_3 = u + c, \quad r_3^\top = (0, \rho, c, 0)$$

$$\lambda_4 = zu, \quad r_4^\top = (0, 0, 0, 1)$$

The fields 1 and 4 are linearly degenerated while the fields 2 and 3 are genuinely non-linear.

Moreover we can write the Rankine-Hugoniot relations for a shock with *non-zero* speed σ :

$$\begin{cases} -\sigma[z] = 0 \\ -\sigma[\rho] + [\rho u] = 0 \\ -\sigma[\rho u] + [\rho u^2 + P] = 0 \\ \begin{cases} -\sigma[v] = 0 & \text{if } \sigma < 0 \\ -\sigma[\rho v] + [\rho uv] = 0 & \text{if } \sigma > 0 \end{cases} \end{cases}$$

For $\sigma = 0$, one has $[\rho u] = [\rho u^2 + P] = 0$, and z may jump. However, Rankine-Hugoniot conditions on the transverse component are undefined. In that case, the 1-field would coincide with a genuinely non linear field.

The Rankine-Hugoniot relations imply that in a shock $[z] = 0$ if and only if $\sigma \neq 0$, that is in the 2-shock, 3-shock and 4-waves. For $\sigma > 0$, the above system provides the equation :

$$\overline{\rho(u - \sigma)}[v] = 0 \tag{3.12}$$

Thus, if $\sigma > 0$, $[v] = 0$ in the 2-shock or 3-shock waves since $\sigma \neq \overline{\rho u}/\bar{\rho}$. If we focus on the 4-wave (contact wave) propagating in the region $x > 0$, we retrieve the trivial solution $\sigma = \bar{u}$ which provides no constraint for v . On the other side, if $\sigma < 0$, the relation $-\sigma[v] = 0$ also implies that $[v] = 0$.

The subset ((3.9),(3.10)) involves u and ρ and is the classical one dimensional isentropic Euler model which gives the solution (u^*, ρ^*) (see figure (3.3) and section 2.2.3). The Riemann invariants of the system are:

$$IR_1 = \{\rho, u, v\}$$

$$IR_2 = \{z, v, u + g(\rho)\}$$

$$IR_3 = \{z, v, u - g(\rho)\}$$

$$IR_4 = \{z, \rho, u\}$$

Since the first field is linearly degenerated and since z is preserved through the 2-wave, the 3-wave and the 4-wave:

$$z(x, y, t) = \begin{cases} z_R = 1 & \text{if } x > 0 \\ z_L = 0 & \text{if } x < 0 \end{cases}$$

Since v is preserved through the 1-wave, the 2-wave and the 3-wave:

$$v(x/t = 0^-) = v_L = 0$$

$$v(x/t = 0^+) = \begin{cases} v^- = v_L & \text{if } \lambda_4 > 0 \\ v_R & \text{if } \lambda_4 \leq 0 \end{cases}$$

We emphasize that the 4-contact wave cannot travel to the left domain because $z(x < 0, y, t) = 0$. This leads to the numerical flux on the ρv -component :

- if $u^* > 0$:

$$(\rho uv)(x/t = 0^-) = 0$$

$$(\rho uv)(x/t = 0^+) = 0$$

– if $u^* < 0$:

$$(\rho v)(x/t = 0^-) = 0$$

$$(\rho v)(x/t = 0^+) = (\rho u)(x/t = 0)v_R$$

Since $(\rho v)(x/t = 0^-)$ is always null, this model respects the (NSC).

Remark 7 *An important point to be quoted is that we obtain the same discrete fluxes using the Godlewski-Raviart method [38],[39] with fluxes:*

$$f_L = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ 0 \end{pmatrix} \text{ and } f_R = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho v \end{pmatrix}$$

Remark 8 *We check now the continuity of $(\rho v)(x/t = 0^\pm)$ with respect to u^* at $u^* = 0$. This is important for the stability of cases which involve states at rest around the interface. Of course, we always have $(\rho v)(x/t = 0^-) = 0$ whatever u^* is. Hence:*

$$\lim_{u^* \rightarrow 0^-} (\rho v)(x/t = 0^-) = 0 = \lim_{u^* \rightarrow 0^+} (\rho v)(x/t = 0^-)$$

We focus now on $(\rho v)(x/t = 0^+)$. First of all, we have:

$$\lim_{u^* \rightarrow 0^+} (\rho v)(x/t = 0^+) = 0$$

We eventually want to prove that $\lim_{u^* \rightarrow 0^-} (\rho v)(x/t = 0^+) = 0$. For that purpose we need to introduce a new variable q and its governing equation:

$$\partial_t (\rho q) + \partial_x (\rho u q) = 0$$

The eigenvalue associated with this new linearly degenerated field is $\lambda_5 = u$ which, unlike $\lambda_4 = zu$, can be negative. This will enable to find the limit of $(\rho v)(x/t = 0^+)$ when u^* tends towards 0^- . This new variable q and its governing equation do not change the structure of the solution for z , ρ , u and v . Since u only varies through the 2-wave and the 3-wave, and since $\lambda_5 = u^*$, we have:

$$\lim_{\lambda_5 \rightarrow 0^-} u(x/t = 0) = \lim_{\lambda_5 \rightarrow 0^-} u(x/t = 0^-) = \lim_{\lambda_5 \rightarrow 0^-} u^* = 0$$

hence,

$$\lim_{u^* \rightarrow 0^-} (\rho v)(x/t = 0^+) = 0$$

3.3.4 A conservative admissible model at the interface

We still use:

$$z = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases}$$

We consider the conservative interface model:

$$\partial_t (z) = 0 \tag{3.13}$$

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \tag{3.14}$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \tag{3.15}$$

$$\partial_t (\rho v) + \partial_x (z \rho v) = 0 \tag{3.16}$$

In the right region ($x/t > 0$) one recovers the projection of the model (3.3). For ($x/t < 0$), (3.15) reads $\partial_t(\rho v) = 0$, and can be integrated, which provides $\rho v(x < 0, t > 0) = 0$ since $v(x < 0, t = 0) = 0$. One thus clearly retrieves the onedimensional model $v(x < 0, t > 0) = 0$ for positive densities (vacuum occurrence is beyond the scope of our approach).

In terms of the non-conservative variables $Y^\top = (z, \rho, u, \rho v)$, the eigenvalues and eigenvectors of the Jacobian matrix associated to the system (3.13)-(3.16) are:

$$\begin{aligned}\lambda_1 &= 0, & r_1^\top &= (z, 0, 0, -\rho v) \\ \lambda_2 &= u - c, & r_2^\top &= (0, \rho, -c, \frac{-\rho v c z}{(u-c)-uz}) \\ \lambda_3 &= u + c, & r_3^\top &= (0, \rho, c, \frac{\rho v c z}{(u+c)-uz}) \\ \lambda_4 &= zu, & r_4^\top &= (0, 0, 0, 1)\end{aligned}$$

The first and fourth fields are linearly degenerated while the second and third fields are genuinely non-linear. Jump conditions are uniquely defined.

An important point to be quoted is that the subset of equations (3.14)-(3.15) does not depend on z or v . Thus the solution of a Riemann problem for (3.13)-(3.16) will give for the pair (ρ, u) the same solution as the Riemann problem for the sole equations (3.14)-(3.15) when considering the same initial condition for ρ and u (see section 2.2.3). Hence, we focus now on the transverse component of the flux.

We first consider the Rankine-Hugoniot relation through the first wave. We have:

$$[\rho u z v] = 0 \quad \text{and} \quad [\rho u] = 0$$

which implies:

$$[z v] = 0 \tag{3.17}$$

(unless $(\rho u)(x = 0, t > 0) = 0$, which does not modify the conclusions). The only Riemann problems that are relevant for our purpose are those for which right and left states comply with:

$$z_L = 0 \quad \text{and} \quad z_R = 1 \quad \text{and} \quad v_L = 0$$

With this initial condition, (3.13) enables to retrieve $z(x < 0, t > 0) = 0$ and $z(x > 0, t > 0) = 1$. Assuming that no resonance phenomenon occurs, the equation (3.17) implies that the transverse velocity at $x/t = 0^+$ is:

$$v^+ = 0$$

Hence the transverse flux at $x/t = 0^+$ for such Riemann problems is:

$$(\rho u z v)^+ = (\rho u v)^+ = 0 \tag{3.18}$$

We may retrieve this simply considering: $[\rho u z v] = 0$, which gives $(\rho u z v)^+ - (\rho u z v)^- = 0$ or $(\rho u z v)^+ = (\rho u z v)^- = 0$. We do not need to assume that $v^- = 0$ to obtain the relation (3.18).

Since $z^- = 0$, we have no information on the "transverse flux" $(\rho u v)$ at $x/t = 0^-$ when focusing on the first wave. We can only conclude that $(\rho u z v)^- = 0$. In order to recover relevant information, we need to consider the half plane $x/t < 0$. The only waves which can develop in the domain

$x/t < 0$ are the two genuinely non-linear waves associated with λ_2 and λ_3 . Since $z(x/t < 0) = 0$, the equation (3.16) reads:

$$\partial_t(\rho v) = 0, \quad \forall(x/t) < 0$$

Hence, if we assume that the left transverse velocity in the initial condition of the Riemann problem is $v_L = 0$, and thus that $\rho_L v_L = 0$, we obtain $(\rho v)^- = 0$. We can conclude that the transverse flux at $x/t = 0^-$ is:

$$(\rho uv)^- = 0 \tag{3.19}$$

This conservative interface model thus respects the (NSC) condition in the frame of a Riemann problem with correct initial condition $v_L = 0$.

3.4 Numerical schemes and results

All methods described herein rely on the Finite Volume method (see [27]). Instead of using the exact Godunov scheme, we apply herein for the approximate Godunov scheme VFRoe-ncv introduced in [16], using the non conservative variable $Y^T = (\rho, u, v)$. We restrict here to the so-called "first-order" scheme. Wall boundary conditions are accounted for by using the standard mirror approach. ([16] and [37]).

3.4.1 The computational domain

The coarse mesh

The above method will be tested on a domain composed of a pipe connected to the middle of the left side ($x = 0$) of a squared tank. The pipe is 2 unit long and $h_0 = \frac{2}{21}$ unit high; the sides of the tank are 2 unit long. The initial mesh (see fig:(3.4)) contains 21×21 regular square cells in the tank and 21 cells in the pipe. Hence all the cells of this initial mesh are squares of the same size $h_0 = \frac{2}{21}$.

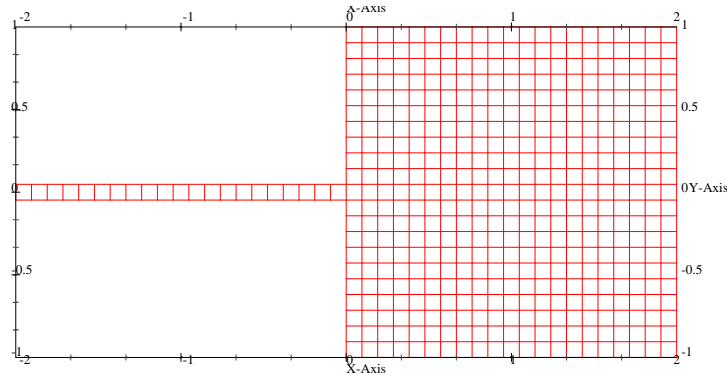


FIG. 3.4 – *The coarse mesh*

Position of the interface

Two different positions for the interface $x_{interf} = \{0, -5h_0\}$, where h_0 is the diameter of the pipe, are used to define the boundary between one- and two-dimensional domains on the initial mesh (see fig:(3.5)). That is, the domain on the left of $x = x_{interf}$ is the one-dimensional domain and the domain on the right is the two-dimensional domain.

Mesh refinement

We use three levels of refinement. The cells of the two-dimensional domain are respectively cut into 2, 4 and 8 in each direction. The one-dimensional domain cells are respectively cut into 2, 4 and 8 in the x direction (see fig:(3.5)). The last cell on the right side of the one-dimensional domain thus has 4, 5, 7 and 11 edges, depending on the mesh level refinement. The finest grid approximately contains 30000 nodes.

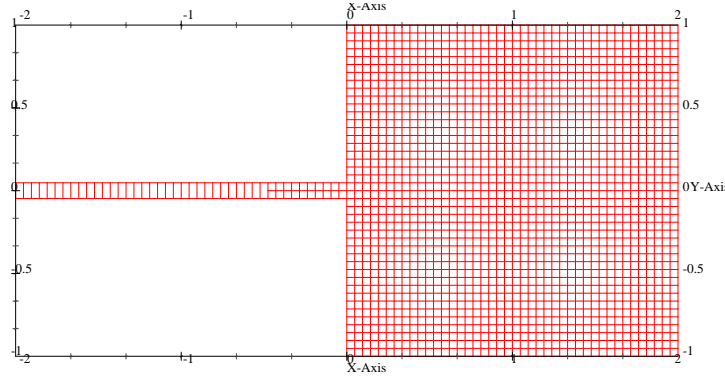


FIG. 3.5 – Example of mesh for $x_{interface} = -5h_0$ and for the first level of refinement

3.4.2 Initial conditions and EOS parameters

We consider herein a Riemann problem derived from the shock tube experiment. As initial conditions, we set ρu and ρv equal to zero on the whole domain and for the density we set:

$$\rho(x,y;t=0) = \begin{cases} \rho_l & \text{if } y > x - 0.15 \\ \rho_r & \text{else.} \end{cases}$$

These initial conditions seem to be the worst configuration to test the coupling methods. Actually, we intend to maximize $(\rho uv)^+$, in order to track possible deficiencies. The most tedious situation appears when the fluid flows from the tank into the pipe with "high" flux component in the y direction.

The EOS for the pressure is the stiffened gas law in isentropic form:

$$P = s_0 \rho^\gamma - P_\infty \quad \text{and} \quad c^2 = \frac{\gamma}{\rho} (P + P_\infty)$$

These EOS allow us to simulate perfect gas with the parameters:

$$P_\infty = 0, \gamma = 1.4 \text{ and } s_0 = 10^6$$

and to approach water behavior using

$$P_\infty = 10^9, \gamma = 2.34 \text{ and } s_0 = 95.51.$$

For gas simulation we have chosen $\rho_r = 0.5$ and $\rho_l = 1$; for water simulation we have chosen $\rho_r = 800$ and $\rho_l = 1000$. The figures (3.6),(3.7),(3.8) and (3.9) show the numerical solution computed for the gas parameters at $t = 2e^{-4}$ on the second level mesh with interface at $x_{interface} = -5h_0$ with our interface model. With these initial conditions a shock wave travels to the left upper corner of the tank, hitting the interface edges, and a rarefaction wave moves to the right lower corner of the tank (the results of figures (3.6),(3.7),(3.8) and (3.9) show the solution computed when the shock wave reaches the left upper corner).

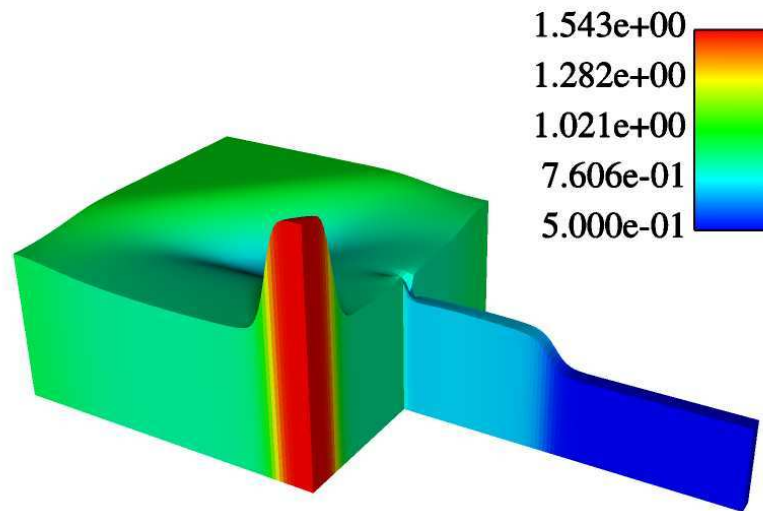


FIG. 3.6 – *density map*

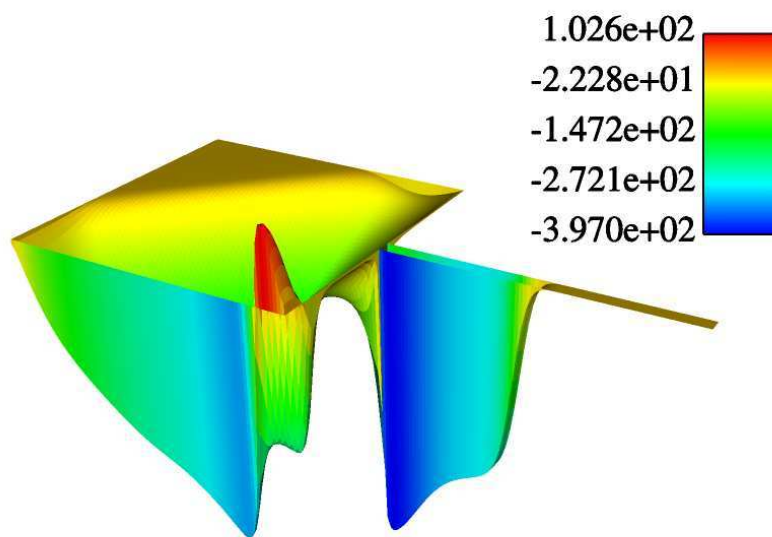


FIG. 3.7 – ρu *x-momentum map*

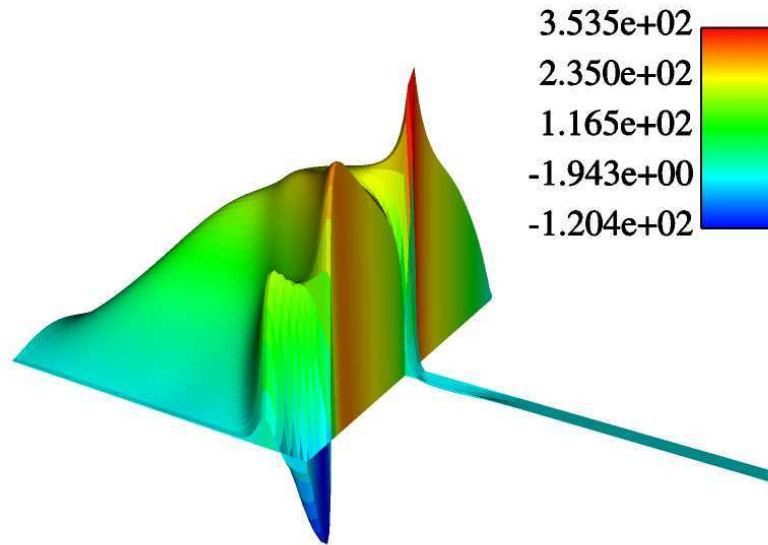


FIG. 3.8 – ρv *y*-momentum map

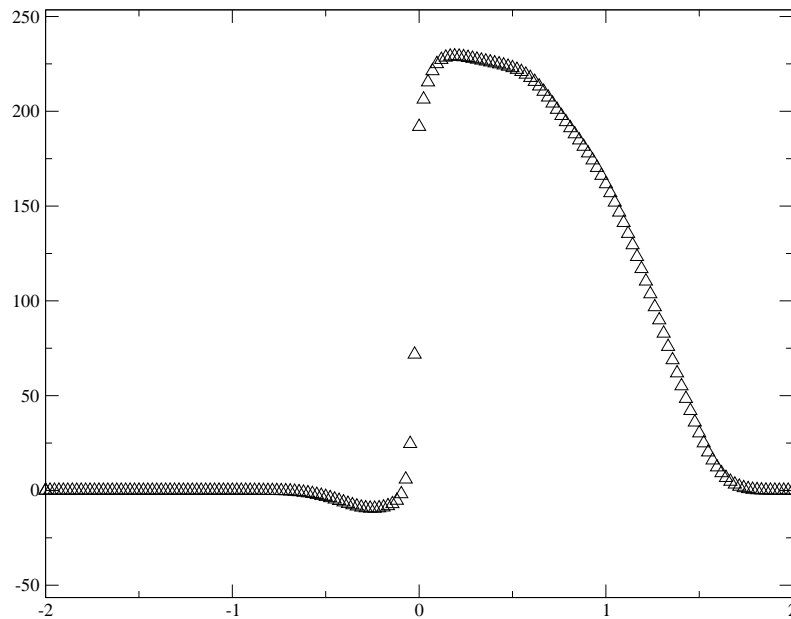


FIG. 3.9 – ρv profile along the line $y = 0$

3.4.3 Numerical fluxes

For both one- and two-dimensional codes we recall that we use the approximate Godunov solver VFRoe-ncv [16] to compute fluxes on each interface between two cells.

We use two different strategies to compute fluxes on both sides of the interface between the 1D code and the 2D code. We recall that (ρ^*, u^*) represent the approximate value on the interface in the solution of the linearized Riemann problem associated with (3.5), (3.6). For all schemes, numerical fluxes $(\rho^* u^*, \rho^* (u^*)^2 + P(\rho^*))$ are of course identical at the coupling interface. Thus the only discrepancies depend on the flux on the (ρv) component.

- The first strategy consists in applying the non-conservative interface model described in the section 3.3, with the VFRoe-ncv scheme, using the variable $Y^\top = (z, \rho, u, v)$. It is referred to in the following as the non-conservative model.

- if $u^* > 0$:

$$(\rho v)^- = 0$$

$$(\rho v)^+ = 0$$

- if $u^* < 0$:

$$(\rho v)^- = 0$$

$$(\rho v)^+ = (\rho u)^* v_R$$

- A second interface scheme is used. This scheme naturally issues from the admissible conservative model which agrees with the (NSC) described in section 3.4. Actually this scheme simply enforces the continuity on the ρv -component of the flux that is:

$$(\rho v)^+ = (\rho v)^- = 0$$

The two other components of the flux are the same as the flux obtained with either the non-conservative model or the conservative model.

3.4.4 Numerical results

As a reference we compute the solution of the two-dimensional model on the whole domain with the finest mesh refinement *in the tank and in the whole pipe*.

The domain can be cut in three subdomains on which errors will be computed separately:

- the tank, $x > 0$.
- the two-dimensional part of the pipe, $0 > x > x_{interf}$ if $x_{interf} < 0$.
- the one-dimensional part of the pipe, $x_{interf} > x$.

Because of the different volumes of the different domains, we will use a normalized L_1 -norm of the error e_1 at time $t^n = T$:

$$e_1(T) = \|(u - u^{ref})(T)\|_{L_1} = \frac{\sum_i |u_i^n - (u^{ref})_i^n| |\Omega_i|}{\sum_i |\Omega_i|}$$

Note that $(u^{ref})_i^n$ does not stand for the exact solution, but for the approximation obtained while using the two dimensional scheme on the finest mesh on the whole computational domain, within cell i and at time t^n .

Remark 9 *The approximate solutions of the component ρv computed with the two interface schemes have null values for the one-dimensional pipe so that the error calculated on this domain is the L_1 -norm of the solution of reference. It is obviously the same for the two schemes.*

The form of the L_1 -norm of the error of the computed solution at the time T on a mesh of size h can be, in a classical manner, expressed as:

$$e_1(h,T) = C(T) \times h^\alpha$$

where the coefficient C is increasing with respect to T . The coefficient α is the rate of convergence of the scheme. We use first order schemes for which $\alpha \in [\frac{1}{2}, 1]$. Actually, when restricting to the linearly degenerated fields, we get $\alpha = \frac{1}{2}$; turning to the genuinely non-linear fields, we have: $\alpha = 1$, and thus if both fields are present in the simulation, α lies in $] \frac{1}{2}, 1[$ (see for instance [31] and [27]).

The figures below represent the ρv -error with respect to $\log \left(\left(\frac{h_0}{2^K} \right)^2 \right)$ (with $K = \{0, 1, 2, 3\}$ the level of refinement) for the two solutions: the non-conservative model is denoted by circles and the conservative model is denoted by squares.

Interface $x_{interface} = 0$

We focus here on the water simulation. (Similar results have been obtained using gas EOS, associated results are given in appendix B). The interface between codes has been placed exactly at the junction between the 1D pipe and the 2D tank. The CFL is fixed to 0.95.

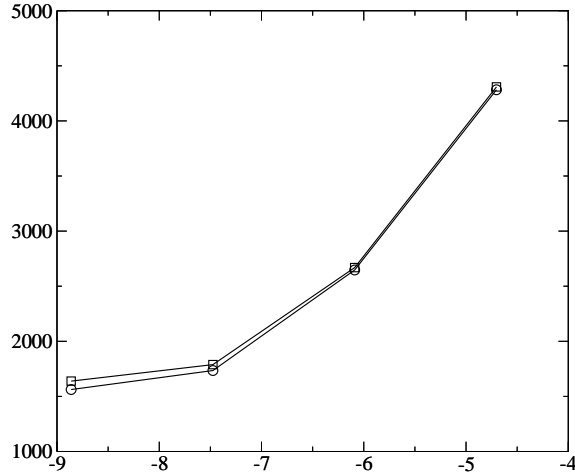


FIG. 3.10 – ρv -error wrt. $\log\left(\left(\frac{h_0}{2K}\right)^2\right)$ in the 2D Tank

Interface $x_{interface} = -5h_0$

We use the same initial conditions, but the interface between codes is now located at $x = -5h_0$. We still use the same CFL time stepping limitation.

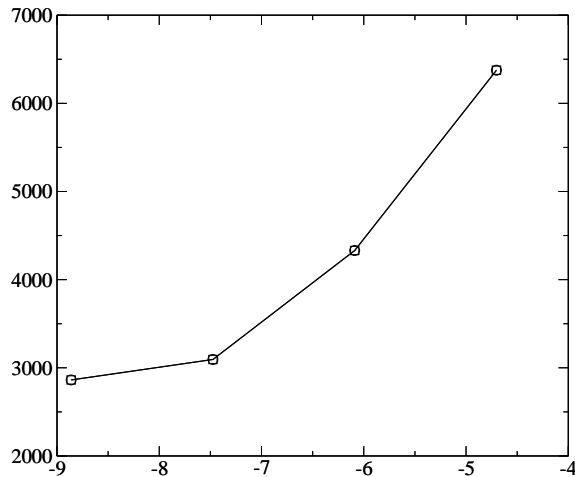


FIG. 3.11 – ρv -error wrt. $\log\left(\left(\frac{h_0}{2K}\right)^2\right)$ in the 2D Tank

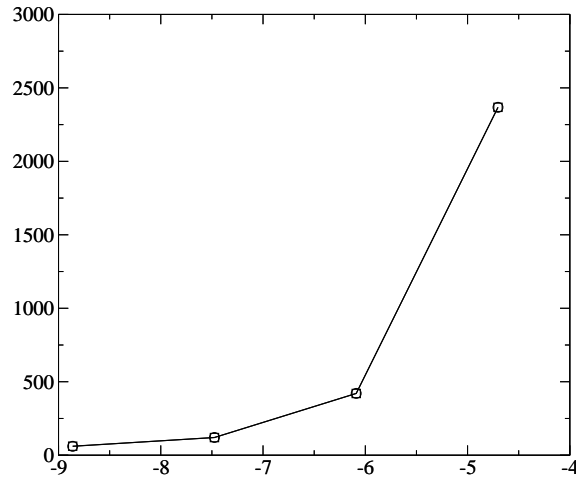


FIG. 3.12 – ρv -error wrt. $\log\left(\left(\frac{h_0}{2K}\right)^2\right)$ in the 2D pipe

Some qualitative results in the pipe direction

We present herein the values of the field $\rho v(x, y = 0)$ (on the line $y = 0$), focusing on the finest mesh ($h = h_0/8$). The squares denote the solution computed with the conservative model, the circles denote the solution for the non-conservative model and the line denotes the reference solution.

For gas simulations, it appears that the L^1 norm of the error is approximately the same for both conservative and non-conservative approaches. Nonetheless, the error is much higher close to the coupling interface when applying for the conservative model, whereas the non-conservative model results are indeed close to those provided by the reference 2D code (see figure (3.13)). *Actually the relative error in the cell close to the right exit of the pipe is about six times larger when using the conservative model.* This is true wherever the interface between the two codes lies (see figure (3.15)). We insist that this still holds true when turning to water simulations, though the discrepancies become smaller (see figures (3.16), (3.18)).

From an engineering point of view, it is almost impossible to distinguish any "spurious" reflected wave in the 2D tank.

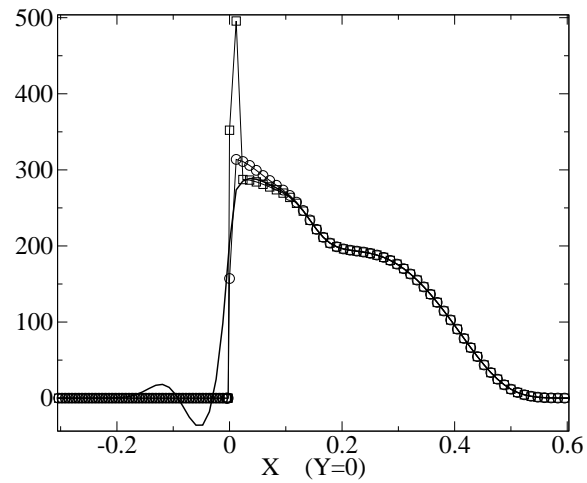


FIG. 3.13 – $\rho v(x, y = 0)$ for gas parameters and $x_{interf} = 0$

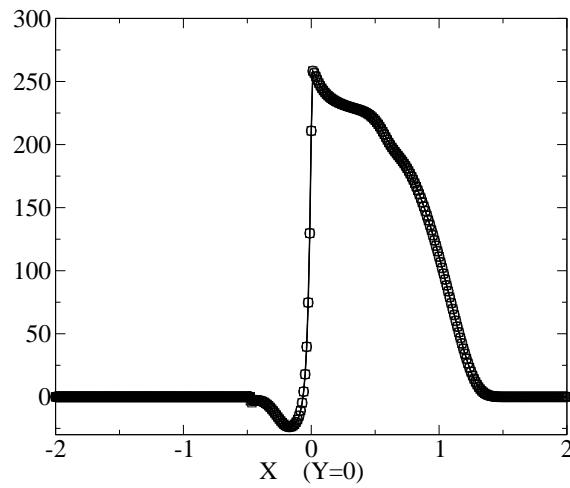


FIG. 3.14 – $\rho v(x, y = 0)$ for gas parameters and $x_{interf} = -5h_0$ (first view)

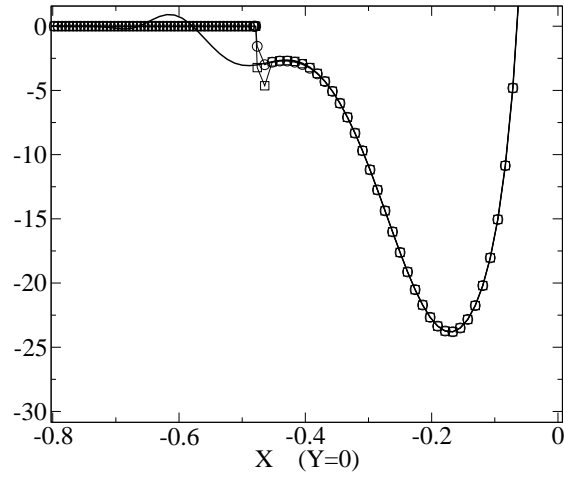


FIG. 3.15 – $\rho v(x, y = 0)$ for gas parameters and $x_{interf} = -5h_0$ (second view)

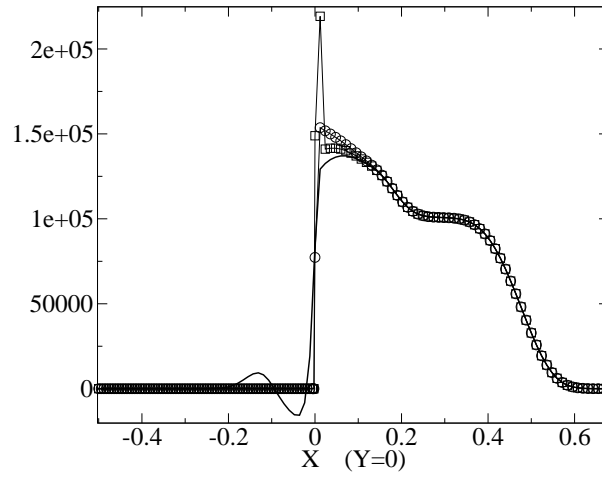


FIG. 3.16 – $\rho v(x, y = 0)$ for water parameters and $x_{interf} = 0$

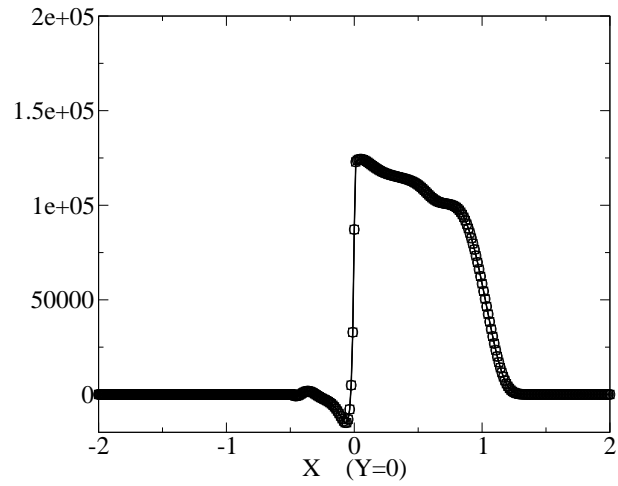


FIG. 3.17 - $\rho v(x, y = 0)$ for water parameters and $x_{interf} = -5h_0$ (first view)

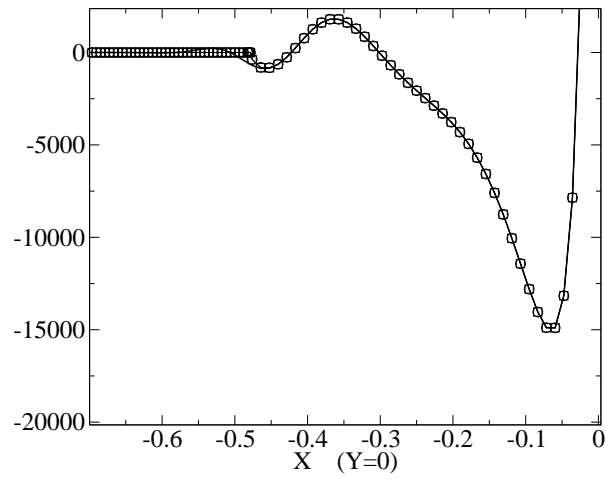


FIG. 3.18 - $\rho v(x, y = 0)$ for water parameters and $x_{interf} = -5h_0$ (second view)

Convergence rate

For each interface scheme, we compute two evaluations of the convergence rate. For that purpose, we use the solutions computed on the two finest meshes and on the two coarsest meshes respectively:

$$\alpha = \text{Log}\left(\frac{e_1(h,T)}{e_1(h/2,T)}\right)/\text{Log}(2)$$

where the choice $h = h_0$ (respectively $h = h_0/4$) provides an approximation of α on the coarse (respectively fine) meshes. Results are given in the following tables.

Convergence rate for the interface $x_{interf} = 0$:

	Non-conservative model		Conservative scheme	
	fine	coarse	fine	coarse
Tank 2D	0.151	0.694	0.126	0.691

Convergence rate for the interface $x_{interf} = -5h_0$:

	Non-conservative model		Conservative scheme	
	fine	coarse	fine	coarse
Tank 2D	0.113	0.558	0.113	0.558

For the latter case $x_{interf} = -5h_0$, we note that the errors are identical, and therefore the approximations of rates of convergence. Actually, (small) discrepancies between computational results only occur in the 2D part of the pipe. This is confirmed when computing similar approximations of rates of convergence *within the part of the pipe on the right side of the coupling interface* (see below).

	Non-conservative model		Conservative scheme	
	finest mesh	coarsest mesh	finest mesh	coarsest mesh
Pipe 2D	601.69	2367.56	612.72	2367.56

Comments

In the 1D part of the pipe, the approximation of v is implicitly set to 0, whereas a meaningful approximation of v arises from the part of the pipe which is simulated with a 2D code. Thus, there exists a *structural part of the global error which is due to the 1D part of the pipe*, independently of the coupling interface and its associated fluxes. This error will in any case be transmitted through the coupling interface. Thus, one expects to retrieve that the L^1 norm of the error computed in the 2D computational domain cannot tend to 0, when the mesh size tends to 0 -unless the coupling interface is moved towards the left end of the pipe-.

– Impact of the coupling technique

As it has already been mentioned, the computational approximations provided by the non conservative model are in better agreement with the true 2D reference results. If one looks at the right side of the coupling interface, a glitch appears when applying for the conservative model, and the amplitude of discrepancies will clearly inhibit the computation of chemical species which are essentially driven by the velocity field. This drawback remains almost unchanged

when the mesh is refined. Such a drawback does not occur when using the non conservative model.

– *Influence of the mesh size*

For coarse meshes, the above estimated rates of convergence α for water simulations seem to lie in $[1/2,1]$, wherever the coupling interface lies. However, for finer meshes which necessarily provide more reliable information, the estimated rates are much lower and close to 0.1 for water simulations. If one turns to gas simulations (see appendix B), this gets worse since it appears that estimated rates of convergence are even lower, when focusing on the finer meshes for instance (the estimation of α is around 0.02). All these values thus confirm that the error in the 2D tank does not go to zero when the mesh is refined.

– *Influence of the coupling interface location*

For a given mesh size, one may push the coupling interface to the left side. Doing so, the meaningful- cell values of v in the 2D part of the pipe (that is on the right side of the coupling interface) naturally tend to vanish. Hence, the approximations provided by both coupling techniques can hardly be distinguished, at least when one focuses on the L^1 norm of the error in the 2D tank; one can nonetheless note slight differences when computing the L^1 norm of the error in the 2D part of the pipe. These results are still in favour of the non conservative coupling technique, and one can retrieve this from a qualitative point of view on figure (3.18).

– *Influence of the EOS*

Though we feel much more concerned by water simulations, it appears that gas simulations enable to retrieve the same patterns. The main difference is probably due to the fact that inertia effects are less important, which makes the computational results closer to those of the 2D reference solution, for a given mesh size, and a given location of the coupling interface (see the first comment above).

3.5 Conclusion

We thus would like to point out that :

(a) the non conservative coupling method proposed herein provides satisfactory results, at least from an engineering point of view ; the conservative coupling technique which agrees with the condition (NSC) generates a bigger pollution around the interface between codes. From an academic point of view, the main advantage of the current framework is that one can examine precisely the amount of error resulting from the "rough" approximation assumed in the 1D code;

(b) the sensitivity to the location of the interface between codes has been examined, which of course confirms *a priori* results. It urges to compute the end of the pipe connected with the 2D/3D tank with a 2D/3D code;

(c) in this particular case of the coupling of a one dimensional code with a two-dimensional code with the same "father" model, the discrete version of our non conservative interface model is similar to the one which would result from the application of ideas from [39] ;

(d) the influence of the EOS does not seem to be significant. However, estimated rates of convergence show that the remark (b) is even more crucial for water simulations ;

(e) the inclusion of finite relaxation time scales, and behind this the coupling of HEM and HRM models for instance, may be achieved using similar ideas ([55], [6], [3]). Different numerical strategies to account for these have been partially investigated in [51], which show that the problem of coupling in the steady and unsteady cases should be distinguished;

(f) a similar companion work on the full Euler equations (that is the coupling of the one-dimensional and two-dimensional Euler equations including the total energy governing equations) even confirms that the main drawback of the admissible conservative model has more annoying consequences, since the pollution around the interface may lead to a blow-up of the code, which is due to the occurrence of negative discrete values of the density (see appendix C and [55]). On the other hand, the admissible non-conservative approach provides satisfactory results which are close to the reference solution.

3.6 Acknowledgements

This work was supported by EDF (Électricité de France), CEA (Commissariat à l'Énergie Atomique), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and FRAMATOME-ANP, in the framework of the NEPTUNE project. Computational facilities were provided by EDF. It has benefited from fruitful discussions with Annalisa Ambroso (CEA), Thierry Gallouet (Université Aix Marseille I, LATP), Christophe Chalons, Frédéric Coquel, Edwige Godlewski, Frédéric Lagoutière, Pierre-Arnaud Raviart and Nicolas Seguin (Université Paris VI, Jacques-Louis Lions laboratory). Reviewers are also acknowledged for their useful comments and suggestions.

3.7 Appendix A : A comparison of three distinct interface models

This appendix is devoted to the comparison of results that have been obtained when using :

- (a) the natural conservative interface model which does not fulfill the (NSC) condition;
- (b) the non-conservative interface model which fulfills the (NSC) condition;
- (c) the conservative interface model which fulfills the (NSC) condition.

All computations have been performed using the same mesh with the finest mesh in the tank. The coupling interface is located at $x = 0$. The crosses correspond to the reference solution computed on a full 2D mesh including the pipe. Schemes associated with strategies (b) and (c) have been detailed in section 4.3. The scheme corresponding to the natural strategy (a) reads:

- if $u^* > 0$: $(\rho v)^+ = (\rho v)^- = 0$
- if $u^* < 0$: $(\rho v)^+ = (\rho v)^- = (\rho u)^* v_R$

We obviously check that strategies (a) and (b) provide similar results in the 2D tank, which was expected since $(\rho v)^+$ is the same for both schemes when $u^* < 0$. Of course cell values for ρv within the pipe are non zero when using (a) whereas cell values obtained with (b) and (c) are null. The error on the first cell in the tank region is almost six times greater when using the conservative approach which fulfills the (NSC) condition, that is (c). The latter does not seem suitable, especially if one aims at computing chemical species.

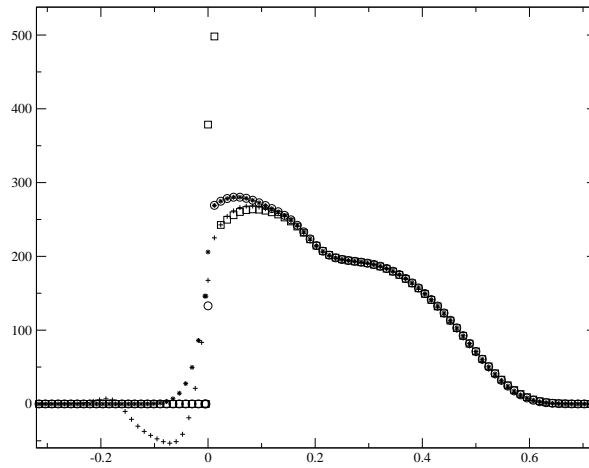


FIG. 3.19 - $\rho v(x, y = 0)$ for gas parameters and $x_{interf} = 0$. stars (a); circles (b); squares (c); crosses (reference 2D solution)

3.8 Appendix B : Error results for the gas simulation

Interface $x_{interf} = 0$

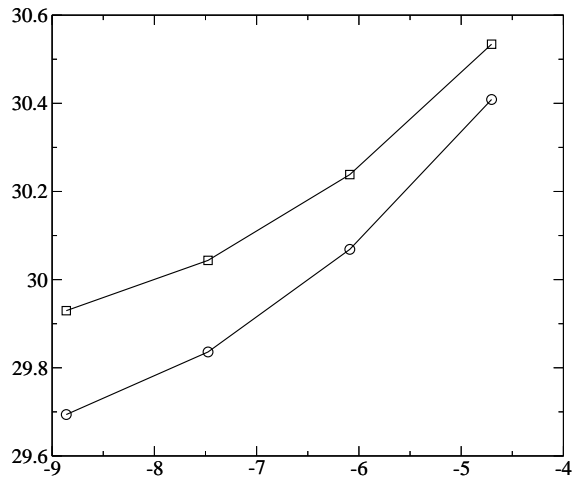


FIG. 3.20 – ρv -error wrt. $\log\left(\left(\frac{h_0}{2K}\right)^2\right)$ in the 2D Tank

Interface $x_{interf} = -5h_0$

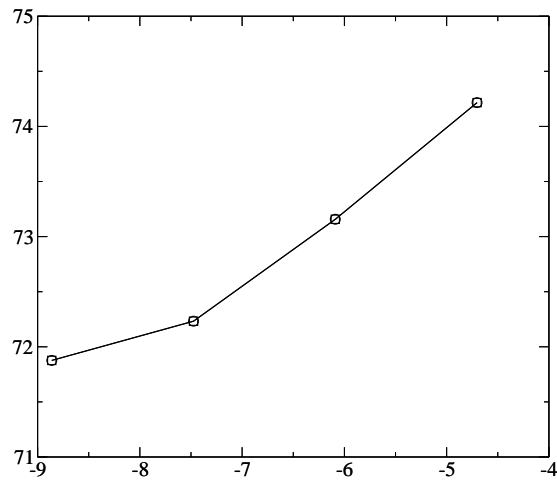


FIG. 3.21 – ρv -error wrt. $\log\left(\left(\frac{h_0}{2K}\right)^2\right)$ in the 2D Tank

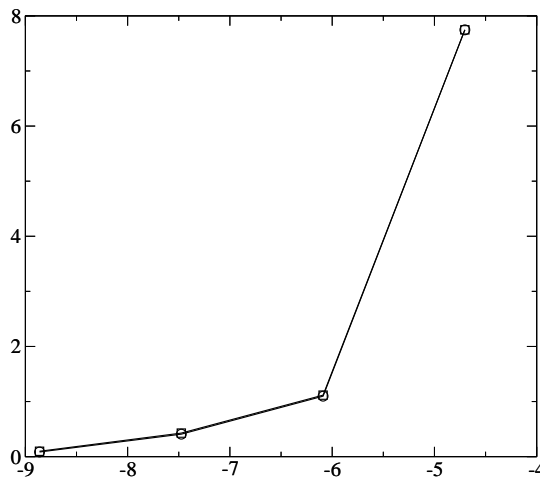


FIG. 3.22 – ρv -error wrt. $\log\left(\left(\frac{h_0}{2K}\right)^2\right)$ in the 2D pipe

3.9 Appendix C : Coupling two and one-dimensional Euler models

In the following we explain how the methods proposed for the Euler system in isentropic form can be applied to the complete Euler system. A numerical test will reinforce the preference for the non-conservative method which respect to the (NSC).

3.9.1 Models to be coupled

Without loss of generality we assume that the interface of coupling is placed along the y -axis at $x = 0$. On the left side of the interface we consider the one-dimensional Euler system:

$$\partial_t (\rho) + \partial_x ((\rho u)) = 0 \quad (3.20)$$

$$\partial_t ((\rho u)) + \partial_x ((\rho u^2 + P)) = 0 \quad (3.21)$$

$$\partial_t (E_1) + \partial_x ((u(E_1 + P))) = 0 \quad (3.22)$$

with,

$$E_1 = \rho e_1(P, \rho) + \rho \frac{u^2}{2}$$

On the right side of the interface we consider the two-dimensional Euler system, the projection of which along the x -axis is (while neglecting transverse derivatives):

$$\partial_t (\rho) + \partial_x ((\rho u)) = 0 \quad (3.23)$$

$$\partial_t ((\rho u)) + \partial_x ((\rho u^2 + P)) = 0 \quad (3.24)$$

$$\partial_t (E_2) + \partial_x ((u(E_2 + P))) = 0 \quad (3.25)$$

$$\partial_t ((\rho v)) + \partial_x ((\rho uv)) = 0 \quad (3.26)$$

with,

$$E_2 = \rho e_2(P, \rho) + \rho \left(\frac{u^2}{2} + \frac{v^2}{2} \right)$$

In the following we will consider that the two models have the same equation of state, that is :

$$e_1(P, \rho) = e_2(P, \rho) = e(P, \rho), \quad \forall (P, \rho)$$

3.9.2 Rewriting the two-dimensional Euler system

We note that the total energy E_2 can be expressed as:

$$E_2 = E_1 + \rho \frac{v^2}{2}$$

The set of equations (3.23)-(3.26) is equivalent to the set of equations (3.27)-(3.30), either for regular solutions or for discontinuities:

$$\partial_t (\rho) + \partial_x ((\rho u)) = 0 \quad (3.27)$$

$$\partial_t ((\rho u)) + \partial_x ((\rho u^2 + P)) = 0 \quad (3.28)$$

$$\partial_t (E_1) + \partial_x ((u(E_1 + P))) = 0 \quad (3.29)$$

$$\partial_t ((\rho v)) + \partial_x ((\rho uv)) = 0 \quad (3.30)$$

An important point to be quoted is that the subset of equations (3.27)-(3.29) does not depend on v . It is the same set of equations than (3.20)-(3.22). We can then apply the methods of flux coupling proposed for the isentropic Euler model.

3.9.3 An interface model for flux coupling

The (NSC) condition keeps its importance in the present case. Hence an interface model is admissible if and only if it respects this condition. We propose herein two models. The definition of the variable z remains unchanged.

A non-conservative admissible interface model

We now consider the following interface model:

$$\partial_t(z) = 0 \tag{3.31}$$

$$\partial_t(\rho) + \partial_x((\rho u)) = 0 \tag{3.32}$$

$$\partial_t((\rho u)) + \partial_x((\rho u^2 + P)) = 0 \tag{3.33}$$

$$\partial_t(E_1) + \partial_x((u(E_1 + P))) = 0 \tag{3.34}$$

$$\partial_t(v) + zu\partial_x(v) = 0 \tag{3.35}$$

This system can not be written in conservative form owing to the non-conservative product $zu\partial_x(v)$. In fact the solution of the Riemann problem is classical for (3.31)-(3.34) (unless some resonance phenomena occurs), but we have to propose a way to solve (3.35). This is achieved using the same idea as developed in the isentropic case. Finally, the numerical fluxes are:

$$F^- = \begin{pmatrix} (\rho u)^* \\ (\rho u^2 + P)^* \\ (u(E_1 + P))^* \\ 0 \end{pmatrix}, \quad F^+ = F^- + \begin{pmatrix} 0 \\ 0 \\ \frac{(\rho u)^*}{2}(v^+)^2 \\ (\rho u)^*v^+ \end{pmatrix}$$

where v^+ is the solution for the variable v at $x/t = 0^+$ and Y^* stands for the exact solution $Y(x/t = 0)$. Obviously the coupling method respects the (NSC) condition and is not conservative.

A conservative admissible interface model

We introduce now a conservative interface model that respects the (NSC) condition. This model is exactly the counterpart of the conservative model proposed for the isentropic case. The governing equations are:

$$\partial_t(z) = 0 \tag{3.36}$$

$$\partial_t(\rho) + \partial_x((\rho u)) = 0 \tag{3.37}$$

$$\partial_t((\rho u)) + \partial_x((\rho u^2 + P)) = 0 \tag{3.38}$$

$$\partial_t(E_1) + \partial_x((u(E_1 + P))) = 0 \tag{3.39}$$

$$\partial_t((\rho v)) + \partial_x((zu\rho v)) = 0 \tag{3.40}$$

Hence the left and right fluxes are:

$$F^- = F^+ = \begin{pmatrix} (\rho u)^* \\ (\rho u^2 + P)^* \\ (u(E_1 + P))^* \\ 0 \end{pmatrix}$$

Thus this model fulfils the (NSC) condition and since $F^- = F^+$ this coupling method is also conservative in terms of total energy.

3.9.4 Numerical results

We use the above methods to simulate the Euler model with perfect gas EOS, that is:

$$(\gamma - 1)\rho e(P, \rho) = P$$

The test case configuration is the same as the one described for the isentropic Euler systems. We choose to present the results obtained for the gas simulation, that is $\gamma = 1.4$. The initial conditions are:

$$\rho(x, y; t = 0) = \begin{cases} 0.5 & \text{if } y > x - 0.15 \\ 1.0 & \text{else.} \end{cases}$$

$$P(x, y; t = 0) = \begin{cases} 10^4 & \text{if } y > x - 0.15 \\ 10^5 & \text{else.} \end{cases}$$

$$u(x, y; t = 0) = v(x, y; t = 0) = 0.0$$

The interface is located in $x = 0$ (i.e. at the connection between the pipe and the tank). All interfacial fluxes are computed using a VFRoe-ncv scheme with the variable $(\rho, u, P, v)^\top$ and the time steps are computed in order to comply with the constraint: $CFL = 1/2$.

The density ρ and the transverse momentum ρv are plotted on the line $y = 0$ (with respect to x). The so-called two-dimensional reference solution is the computation obtained using the two-dimensional Euler model on the whole domain with the mesh refined in all directions. The results which are displayed result from the finest mesh. For the conservative admissible model the overshoot of the transverse velocity makes the computation stop (the density in at least one cell becomes negative). Results are plotted at the last time step before this blow-up occurs.

Moreover, when compared with the conservative admissible model (represented by squares on figures), we observe that results obtained with the non-conservative admissible model (represented by circles on figures) are much closer to the 2D reference solution (represented by crosses on figure) near the coupling interface.

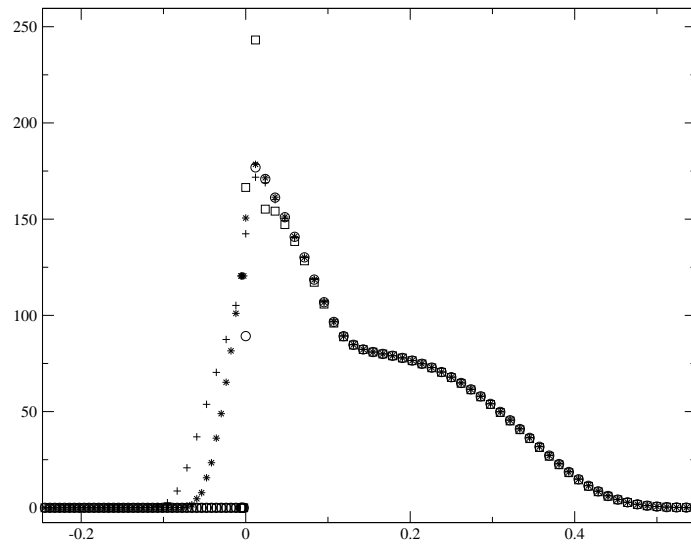


FIG. 3.23 – Solution for the transverse momentum ρv on the line $y=0$. Crosses stand for the two-dimensional reference solution, stars stand for the natural interface model (which does not respect the (NSC)), circles stand for the non conservative admissible interface model and squares stand for the conservative admissible interface model.

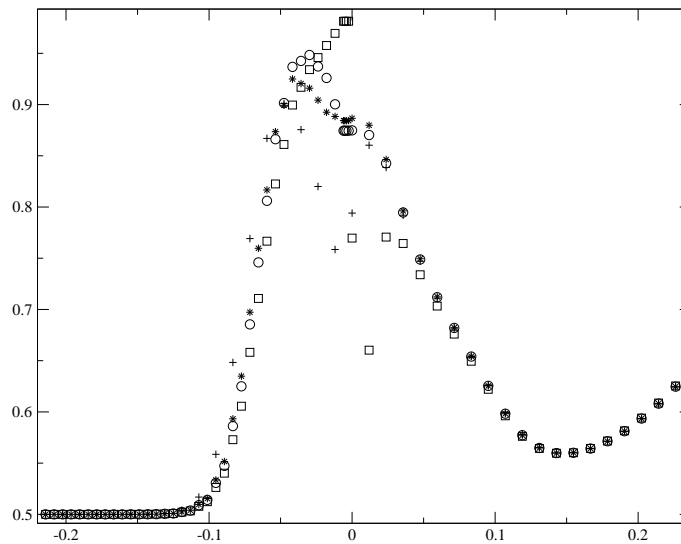


FIG. 3.24 – Solution for the density on the line $y=0$. Crosses stand for the two-dimensional reference solution, stars stand for the natural interface model (which does not respect the (NSC)), circles stand for the non conservative admissible interface model and squares stand for the conservative admissible interface model.

Chapitre 4

Une méthode pour coupler deux modèles diphasiques homogènes de thermohydraulique nucléaire

Lorsque l'on désire coupler des modèles différents, on est amené à considérer des modèles thermodynamiquement différents. Pour décrire un même écoulement plusieurs choix de modèles sont possibles. Ces modèles possèdent des systèmes avec plus ou moins d'équations et donc décrivent de manière plus ou moins fine les phénomènes physiques. Le choix d'un modèle "grossier" se justifie aisément par le gain qu'il apporte d'un point de vue du temps de calcul, à précision sensiblement équivalente au modèle "supérieur" ; autrement dit, à temps de calcul identique, un modèle grossier permettra donc d'effectuer des calculs sur des maillages plus fins qu'un modèle plus fin.

Nous avons choisi de coupler un modèle homogène relaxé (HRM) et un modèle homogène équilibré (HEM). Ces modèles décrivent des écoulements diphasiques, le premier étant directement issu du modèle bi-fluide standard (modèle mono-pression à six équations). Leurs systèmes d'équations font intervenir des grandeurs de mélange qui sont des moyennes des grandeurs phasiques correspondantes. Celles-ci sont la densité du mélange, la vitesse du mélange et l'énergie totale du mélange pour HEM ; le modèle HRM possède les mêmes variables auxquelles on ajoute le titre masse de liquide. Alors que dans le modèle HEM les grandeurs thermodynamiques respectent un *équilibre thermodynamique local instantané* de façon implicite, dans le modèle HRM une échelle de temps finie permet de se rapprocher d'un tel équilibre en jouant sur le titre liquide.

Pour déterminer le système d'équations du modèle HRM nous avons suivi la méthodologie Flica et Thyc, qui se base sur le système standard bi-fluide à une pression. De même la fermeture thermodynamique de type Flica/Thyc a été conservée : la phase vapeur est considérée comme étant toujours à saturation. Ceci a une grande influence sur le comportement du modèle car avec cette hypothèse on favorise les écoulements à faible taux de vapeur. Cela est néanmoins cohérent avec l'utilisation du modèle pour les codes simulant les écoulements dans le circuit primaire de la centrale. Les termes de *drift*, liés à la différence de vitesse des deux phases, n'ont pas été pris en compte pour mettre l'accent sur le couplage thermodynamique. En effet, certains modèles de drift peuvent avoir des conséquences néfastes sur le domaine d'hyperbolicité. En outre la simplification des tables thermodynamiques eau-vapeur (lois analytiques) permettra une étude théorique partielle des deux modèles. Le modèle HEM est quant à lui celui utilisé dans le code Thyc. Les équations sur les gran-

deurs moyennées sont semblables aux équations d'Euler. Les lois de fermeture utilisent la même table thermodynamique que le modèle HRM.

La méthode de couplage que nous avons appliquée pour mettre en relation un code basé sur le modèle HEM et un code basé sur le modèle HRM est une variante de la méthode de couplage par flux utilisée au chapitre précédent. Un modèle d'interface adéquat permet de calculer des flux qui sont transmis comme conditions aux limites aux codes de par et d'autre de l'interface de couplage. Nous introduisons une variable caractéristique du domaine, notée Y , qui prend la valeur 1 dans le domaine HRM et 0 dans le domaine HEM. L'introduction d'une onde de contact stationnaire $\partial_t Y = 0$ (méthode retenue au chapitre précédent) signifie que les deux domaines ne bougent pas. Ceci peut entraîner des problèmes de résonance si le "fan" d'une onde de détente contient la droite $x/t = 0$. L'équation $\partial_t Y = 0$ est remplacée par l'équation de convection-relaxation :

$$\partial_t(\rho Y) + \partial_t(\rho U Y) = \lambda \rho (Y_0 - Y) \quad \text{avec} \quad \lambda = +\infty$$

Cette équation est traitée numériquement en séparant la partie convective et le terme source (voir le premier chapitre). Ainsi elle autorise temporairement et fictivement le déplacement de la frontière entre les deux domaines (partie convective), puis rectifie instantanément ce déplacement (relaxation de Y vers sa valeur initiale Y_0). La structure des ondes du système d'Euler est donc conservée, évitant ainsi les superpositions d'ondes.

Des tests numériques ont été menés afin de détecter la pollution générée par la méthode de couplage. Pour cela nous avons successivement envoyé sur l'interface entre les codes des ondes de contact, des ondes de détente et des ondes de choc. Les conditions initiales ont été choisies afin de recréer les conditions de fonctionnement du coeur d'une centrale nucléaire. A l'issue de ces tests il s'avère que la méthode de couplage proposée présente de bonnes propriétés dont certaines sont liées aux propriétés des modèles HEM et HRM. L'utilisation du schéma numérique VFRoe-ncv en variable (ρ, U, P) pour HEM et (C, ρ, U, P) pour la partie convective de HRM, ainsi que la forme des énergies internes des deux modèles, permettent la préservation d'une partie des solutions de type discontinuité de contact dans chacun des domaines (en l'absence de terme source bien sûr). Le schéma de couplage autorise, dans certains cas, le passage de ces ondes sans aucune pollution dans le sens HEM vers HRM. Un deuxième point positif est la bonne stabilité du schéma de couplage. En effet tous les arrêts du code de calcul sont liés au fait que les grandeurs de maille calculées sortent du domaine de définition des lois thermodynamiques. Dans la majorité des configurations testées, la pollution générée reste acceptable. Un cas test reproduisant schématiquement la mise en fonctionnement du coeur d'une centrale est présenté, les ondes de chocs générées par la mise en chauffe du réfrigérant étant transmises par l'interface de couplage sans pollution excessive.

A method to couple two-phase flow models

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Abstract : We present a method for the unsteady coupling of two distinct two-phase flow models (namely the Homogeneous Relaxation Model, and the Homogeneous Equilibrium Model) through a thin interface. The basic approach relies on recent works devoted to the interfacial coupling of CFD models, and thus requires to introduce an interface model. Many numerical test cases enable to investigate the stability of the coupling method.

4.1 Introduction

We focus in this report on the unsteady interfacial coupling of two distinct two-phase flow models that are commonly used in order to simulate water-vapour flows in nuclear power plants. The main objective here is to derive suitable boundary conditions for both codes associated with HEM and HRM models.

The Homogeneous Relaxation Model (denoted by the acronym HRM) is a four-equation model that is widely used in two-phase flow simulations. Most industrial codes within the nuclear community - for instance THYC (EDF) or FLICA (CEA) - rely on this model. This model requires computing approximations of solutions of two mass balance equations, a total momentum equation and a governing equation for the total energy balance of the mixture. Let alone of source terms, this model is under conservative form. The sole non-zero source contribution is on the right side of the governing equation of the liquid mass fraction. This source tends to relax the current liquid mass fraction to the equilibrium mass fraction, which only depends on the mean pressure and the mean density. The underlying time scale is highly variable, and in practice it makes the source term very stiff, which may render the computation of the HRM model rather uneasy. Actually, the Homogeneous Equilibrium Model (acronym HEM) precisely stands for the counterpart of the HRM model when *an equilibrium is achieved*. It is thus a pure convective set of partial differential equa-

tions which govern the motion of the total mass, the global momentum and the total energy of the whole mixture. Both the HEM and the HRM models require defining appropriate equations of state (referred to as the EOS in the following) in order to account for both the "pure vapour" phase, the "pure liquid" phase but also the "mixture" phase. These EOS are usually tabulated (see[65, 77, 45]), but we will focus here on simplified analytical EOS. This is essentially motivated by the fact that we wish not to mix numerical drawbacks due to the use of realistic EOS and those connected with the formulation of the coupling techniques. In other words, we want to be "optimal" in some sense in terms of EOS in order to concentrate on the main drawbacks of the coupling techniques.

Quite recently, some authors have proposed three approaches in order to tackle the unsteady interfacial coupling of CFD models. Roughly speaking, the first two rely on basic ideas introduced in[44, 38] , whereas the third one takes its grounds on the use of relaxation methods[26, 14, 15] . The coupling technique that is used herein is somewhat equivalent to the one described in[6, 4] , which differs from those investigated in[8, 49, 38, 52, 39] . We want here to take advantage of the fact that the HRM model may be viewed as the father's model of the HEM model. Another advantage of the present approach is that one may get rid of possible resonance phenomena, as underlined in[4] for instance. Though it is not clear whether this has drastic consequences, it seems indeed much appealing to avoid this problem that is not clearly understood ([36]) .

The paper is thus organized as follows:

- Sections II and III are devoted to the presentation of both HEM and HRM models, but also on some of their properties (hyperbolicity, entropy inequality, positivity results for smooth enough solutions).
- We then present the coupling method in section IV. Special attention will be paid to the numerical treatment of the coupling interface, which relies on:
 - (i) an evolution step,
 - (ii) an instantaneous relaxation step,
 - (iii) a finite relaxation step in order to account for source terms.

This section also includes a brief description of the Finite Volume methods that will be applied in order to compute approximations of solutions in non coupled codes.

- Numerical results are displayed in section V. This includes basic test cases involving contact waves, shock waves and rarefaction waves, but also a schematic representation of the flow in a part of the primary coolant circuit in a nuclear power plant.

4.2 The Homogeneous Relaxation Model

This four-equation model can be derived from the six-equation two-fluid model. In the following we focus on specific closure laws and we detail some properties connected with these choices.

Throughout the paper, we will use the following notations. ρ stands for the density of the mixture, $\tau = 1/\rho$, U represents the mean velocity of the mixture. Moreover P , C , e , $h = e + P/\rho$, $E = e + U^2/2$ respectively stand for the pressure, the liquid mass fraction, the internal energy, the enthalpy, and the total volumetric energy of the mixture. The subscripts v and l respectively refer to the *vapour* and the *liquid* phases. The over-script s denotes some saturated quantity.

4.2.1 Closure laws

We consider that the two fluids have the same velocity, that is $U_l - U_v = U_R = 0$. In order to take into account the mass transfer between the two phases, a source term $\rho\Gamma$ stands on the right hand side in the equation of the liquid phase. Thus the governing equations are:

$$\begin{cases} \partial_t(\rho C) + \partial_x(\rho C U) = \rho\Gamma \\ \partial_t(\rho) + \partial_x(\rho U) = 0 \\ \partial_t(\rho U) + \partial_x(\rho U^2 + P) = 0 \\ \partial_t(\rho E) + \partial_x(U(\rho E + P)) = 0 \end{cases} \quad (4.1)$$

with:

$$E = e_{HRM}(P, \rho, C) + \frac{U^2}{2} \quad \text{and} \quad e_{HRM}(P, \rho, C) = h_{HRM}(P, \rho, C) - \frac{P}{\rho}$$

In the following, the HRM model will refer to the set of equations (4.1) with the following definitions of e_{HRM} , Γ and the saturation curves. The set of physical relevant states is:

$$\Omega_{HRM} = \{(\rho, U, P, C) / \rho \geq 0, C \in [0, 1], P \geq 0\}$$

The source term Γ depends on the density ρ , the pressure P and the liquid mass fraction C . It involves a positive time scale τ_0 . We must now specify the form of the enthalpy function h_{HRM} in order to close the system. We choose the thermodynamic closures inspired by the THYC and FLICA codes[77, 45]:

$$\rho h_{HRM}(P, \rho, C) = \rho C h_l(P, \rho_l) + \rho(1 - C) h_v^s(P) \quad (4.2)$$

and

$$\rho_l = \rho C \frac{1}{1 - \rho(1 - C)\tau_v^s(P)} = \frac{C}{\tau - (1 - C)\tau_v^s(P)}$$

The gas is always in a saturation state. In order to get rid of cumbersome computations, we also assume in this work that the equations of state (EOS) within each pure phase are perfect gas EOS. We note $\gamma_l > 1$ (respectively $\gamma_v > 1$) the adiabatic constant for the liquid (respectively the vapour). We recall that the following relation holds:

$$(\gamma_p - 1)\rho e_p = P \quad \text{or} \quad h_p = \delta_p P \tau \quad \text{with} \quad \delta_p = \gamma_p / (\gamma_p - 1)$$

for $p = l, v$. Thus the liquid enthalpy h_l in the equation (4.2) becomes,

$$h_l(P, \rho) = \frac{\delta_l P}{\rho}$$

We will use standard values in order to account for liquid and gas respectively: $\gamma_l = 1.001$ and $\gamma_v = 1.4$. Moreover, we also assume that if the pressure P stays in $[P_{MIN}, P_{MAX}]$ the saturation curves for the enthalpy and the volumetric fraction can be approached by the following functions:

– Saturated vapour:

$$h_v^s(P) = A_v P + B_v \quad \text{and} \quad \tau_v^s(P) = \frac{h_v^s(P)}{\delta_v P} \quad (4.3)$$

– Saturated Liquid

$$h_l^s(P) = A_l P + B_l \quad \text{and} \quad \tau_l^s(P) = \frac{h_l^s(P)}{\delta_l P} \quad (4.4)$$

The coefficients A_v , A_l , B_v and B_l can be found below.

Hence, the enthalpy of the model can be simplified, by accounting for (4.3).

$$\rho h_{HRM}(P, \rho, C) = \delta_l P + \rho(1 - C)h_v^s(P)\left(1 - \frac{\delta_l}{\delta_v}\right) \quad (4.5)$$

This simplified form of EOS will enable to derive some technical results.

The source term Γ in the set of equations (4.1) allows the exchange of mass between the two phases. Its form arises from the literature:

$$\Gamma = \frac{C(1 - C)}{\tau_0} \rho \tau_v^s(P) \frac{h_l^s(P) - h_l(P, \rho_l)}{h_v^s(P) - h_l^s(P)} \quad (4.6)$$

where τ_0 is a time scale.

4.2.2 Hyperbolicity of the HRM model

In order to study the hyperbolicity of the HRM model, we focus on the convective part of (4.1). Then the non-conservative equations on ρ , U , P and C are:

$$\partial_t \begin{pmatrix} C \\ \rho \\ U \\ P \end{pmatrix} + \begin{pmatrix} U & 0 & 0 & 0 \\ 0 & U & \rho & 0 \\ 0 & 0 & U & \tau \\ 0 & 0 & \hat{\gamma}_{HRM} P & U \end{pmatrix} \partial_x \begin{pmatrix} C \\ \rho \\ U \\ P \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (4.7)$$

with:

$$\hat{\gamma}_{HRM} P = (\partial_P(e_{HRM}))^{-1} \left(\frac{P}{\rho} - \rho \partial_\rho(e_{HRM}) \right)$$

The eigenvalues and eigenvectors of the matrix of the system (4.7) can be found in Appendix 1 (section B). The system is hyperbolic if and only if $\hat{\gamma}_{HRM} P > 0$. We classically define the sound velocity a_{HRM} by:

$$\rho a_{HRM}^2 \stackrel{def}{=} \hat{\gamma}_{HRM} P \quad (4.8)$$

Using the definition (4.5) of h_{HRM} together with the relation $\rho e_{HRM} = \rho h_{HRM} - P$ we can obtain:

$$\left(\frac{P}{\rho} - \rho \partial_\rho(e_{HRM}) \right) = \frac{\delta_l P}{\rho}$$

$$\partial_P (e_{HRM}) = \tau(\delta_l - 1) + (1 - C)\left(1 - \frac{\delta_l}{\delta_v}\right) \frac{d}{dP} h_v^s(P)$$

The term $\frac{\delta_l P}{\rho}$ is always positive, and a sufficient condition for $\partial_P (e_{HRM})$ to be positive is to have,

$$\left(1 - \frac{\delta_l}{\delta_v}\right) \frac{d}{dP} h_v^s(P) > 0$$

Thanks to (4.3), $\frac{d}{dP} h_v^s(P) = A_v$, which is negative for our domain of interest (see numerical values in section V, equation (4.32)) Thus a sufficient condition for $\partial_P (e_{HRM})$ to be positive is:

$$1 < \gamma_l < \gamma_v$$

With the above condition, the system (4.7) is hyperbolic for all $P \in [P_{MIN}, P_{MAX}]$, $\rho > 0$, $C \in [0, 1]$. We insist that this is not a necessary condition.

4.2.3 Some positivity results

Preliminary remark:

We have introduced the source term:

$$\Gamma = \frac{C(1 - C)}{\tau_0} G_1(P, \rho, C)$$

with

$$G_1(P, \rho, C) = \rho \tau_v^s(P) \frac{h_l^s(P) - h_l(P, \rho_l)}{h_v^s(P) - h_l^s(P)}$$

We can rewrite Γ in a form which will appear to be more convenient:

$$\Gamma = (1 - C) (\bar{C} - C) \frac{G_2(P, \rho)}{\tau_0} \quad (4.9)$$

with $G_2 > 0$ if P in $[P_{MIN}, P_{MAX}]$ and $\rho > 0$:

$$G_2(P, \rho) = \rho \tau_v^s \delta_l P \frac{\tau_v^s(P) - \tau_l^s(P)}{h_v^s(P) - h_l^s(P)} \quad \text{and} \quad \bar{C} = \frac{\tau_v^s(P) - \tau}{\tau_v^s(P) - \tau_l^s(P)} \quad (4.10)$$

Hence the ODE

$$\partial_t (C) = \Gamma(P, \rho, C)$$

has two poles. The pole $C = 1$ is repulsive and the pole $C = \bar{C}$ is attractive. The expression of the second pole will make sense for the HEM model.

Positivity results:

We now want to highlight some properties of positivity of the regular solutions of (4.1):

$$\begin{cases} \partial_t (C) + U \partial_x (C) = \Gamma \\ \partial_t (\rho) + U \partial_x (\rho) + \rho \partial_x (U) = 0 \\ \partial_t (U) + U \partial_x (U) + \frac{1}{\rho} \partial_x (P) = 0 \\ \partial_t (P) + U \partial_x (P) + \hat{\gamma} P \partial_x (U) = -\Gamma \frac{\partial_C (e_{HRM})}{\partial_P (e_{HRM})} \end{cases} \quad (4.11)$$

The demonstration of the following results can be found in Appendix 4. If we assume that $U \in L^\infty$ and $Div(U) \in L^\infty$ then,

$$\rho \geq 0$$

Moreover if we assume that $\rho \in L^\infty$ and that P remains in $[P_{MIN}, P_{MAX}]$,

$$C \leq 1$$

and if the additional condition $\bar{C} \geq 0$ is fulfilled then:

$$C \geq 0$$

Nonetheless nothing ensures that \bar{C} remains in $[0,1]$, nothing ensures that P remains in $[P_{MIN}, P_{MAX}]$, and nothing ensures that ρ_l will remain positive.

The domain of validity of our model is then:

$$D_{HRM} = \{C \in [0,1], P \in [P_{MIN}, P_{MAX}], \tau \geq (1 - C)\tau_v^s(P), \rho \geq 0\}$$

Remark 10 *An analytical solution of the HRM model can go out of the domain D_{HRM} . It is thus possible for a "consistent and stable numerical approximation" to go out of D_{HRM} . In practice, if a numerical solution does not remain in this domain the computations will be stopped.*

4.2.4 Entropy and source terms

In this section we wonder whether the source term Γ contributes to the entropy dissipation. We use the classical method of the vanishing viscosity (see for example[37]) .

From the non-conservative form (4.7) of the HRM model we can deduce that the classical entropy pair $(\eta_{HRM}, F_\eta^{HRM})$ agrees with diffusive source terms.

$$\eta_{HRM} = -\rho \ln(S_{HRM})$$

$$F_\eta^{HRM} = U \eta_{HRM}$$

Where $(P, \rho, C) \mapsto S_{HRM}(P, \rho, C)$ stands for the "physical entropy" defined by the PDE:

$$\hat{\gamma}_{HRM} P \partial_P (S_{HRM}) + \rho \partial_\rho (S_{HRM}) = 0 \quad (4.12)$$

It provides the entropy inequality:

$$\partial_t (\eta_{HRM}) + \partial_x (F_\eta^{HRM}) \leq 0 \quad (4.13)$$

We now focus on the non-conservative form of the HRM model with the zero-order source term (4.11). We obtain the equation:

$$\partial_t (\eta_{HRM}) + \partial_x (F_\eta^{HRM}) = \Gamma_\eta$$

with:

$$\Gamma_\eta = \Gamma \frac{\rho}{S_{HRM}} \partial_P (S_{HRM}) \left[\frac{\partial_C (S_{HRM})}{\partial_P (S_{HRM})} - \frac{\partial_C (e_{HRM})}{\partial_P (e_{HRM})} \right]$$

In order to comply with the entropy inequality (4.13), the source term should agree with the relation,

$$\Gamma_\eta \leq 0$$

The definition of the "physical entropy" (4.12) provides:

$$S_{HRM} = Pf(\rho, C)$$

with:

$$\frac{f(\rho, C)}{f_0(C)} = \left(1 + \rho(1 - C)\frac{\beta}{\delta_l - 1}\right)^{\gamma_l} \left(\frac{1}{\rho}\right)^{\gamma_l}$$

and,

$$\beta = \left(1 - \frac{\delta_l}{\delta_v}\right)A_v$$

The positive function $f_0(C)$ should fulfill: $f_0(1) = 1$, thus for $C = 1$ (i.e. in the pure liquid domain) the entropy S_{HRM} takes a classical form for HRM model with one single phase which is governed by a perfect gas law. Hence the above condition turns to be:

$$\Gamma \left[\frac{\partial_C (S_{HRM})}{\partial_P (S_{HRM})} - \frac{\partial_C (e_{HRM})}{\partial_P (e_{HRM})} \right] < 0$$

Of course, using the expression of $S_{HRM} = Pf(\rho, C)$ above, one can check that the form of the source term Γ does not necessarily satisfy the constraint. This may be easily explained: the source term Γ has been picked up from the standard two-phase flow literature, whatever the EOS of the mean fluid is, which may result in a potential conflict. In practice, if one retains $f_0(C) = 1$, the agreement will occur if and only if the source term Γ is positive, that is when the vapour condenses.

4.3 The Homogeneous Equilibrium Model

4.3.1 Governing equations

The Homogeneous Equilibrium Model is governed by a set of three equations in order to account for total mass, total momentum and total energy balances. These read:

$$\begin{cases} \partial_t(\rho) + \partial_x(\rho U) = 0 \\ \partial_t(\rho U) + \partial_x(\rho U^2 + P) = 0 \\ \partial_t(\rho E) + \partial_x(U(\rho E + P)) = 0 \end{cases} \quad (4.14)$$

with:

$$E = e_{HEM}(P, \rho) + \frac{U^2}{2} \quad \text{and} \quad e_{HEM}(P, \rho) = h_{HEM}(P, \rho) - \frac{P}{\rho}$$

On the basis of [4], we know that small discrepancies among EOS may result in rather high differences in results. We thus assume that both EOS are compatible in the following sense. We need to introduce first some function $C_{eq}(P, \rho)$ as follows:

$$C_{eq}(P, \rho) \stackrel{def}{=} \frac{\tau_v^s(P) - \tau}{\tau_v^s(P) - \tau_l^s(P)} \quad (4.15)$$

Remark 11 *It is important to note that $C_{eq}(P, \rho) = \bar{C}$.*

We also need to introduce three subdomains:

- the pure gas domain $D_v = \{\tau > \tau_v^s(P), P \in [P_{MIN}, P_{MAX}]\}$,
- the pure liquid domain $D_l = \{\tau < \tau_l^s(P), P \in [P_{MIN}, P_{MAX}]\}$
- the two-phase region $D_{2\phi} = \{\tau_l^s(P) \leq \tau \leq \tau_v^s(P), P \in [P_{MIN}, P_{MAX}]\}$.

The pure vapour domain (corresponding to $C_{eq} \leq 0$ or equivalently $\tau_v^s(P) \leq \tau$) is not useful for our purpose. In order to complete (4.14), it remains now to define the enthalpy $h_{HEM}(P, \rho)$ on the pure liquid domain and on the two-phase domain:

- If $0 \leq C_{eq} \leq 1$ or equivalently $\tau_l^s(P) \leq \tau \leq \tau_v^s(P)$ (two-phase domain $D_{2\phi}$):

$$h_{HEM}(P, \rho) \stackrel{def}{=} C_{eq} h_l(P, \rho_l(P, \rho, C_{eq})) + (1 - C_{eq}) h_v^s(P)$$

- If $C_{eq} > 1$ or equivalently $\tau_l^s(P) > \tau$ (pure liquid domain D_l):

$$h_{HEM}(P, \rho) \stackrel{def}{=} h_l(P, \rho)$$

We recall the definitions of $h_l(P, \rho)$ and $\rho_l(P, \rho, C)$:

$$h_l(P, \rho) \stackrel{def}{=} \frac{\delta_l P}{\rho}$$

$$\rho_l(P, \rho, C) = \rho C \frac{1}{1 - \rho(1 - C)\tau_v^s(P)}$$

We note that with this definition, we get: $\rho_l(P, \rho, C = C_{eq}) = 1/\tau_l^s(P)$. Hence the enthalpy of the HEM model in the two-phase domain $D_{2\phi}$, simply reads:

$$h_{HEM}(P, \rho) = C_{eq} h_l^s(P) + (1 - C_{eq}) h_v^s(P) \quad (4.16)$$

The enthalpy h_{HEM} is continuous at the boundary between the two domains D_{HEM} and D_l (i.e. continuous at $C_{eq} = 1$). Nevertheless, its derivatives are not continuous.

In the following, the HEM model will refer to the set of equation (4.14) with the above definitions of e_{HEM} and the saturation curves.

Remark 12 *There is a compatibility of the EOS of the HEM model with the EOS of the HRM model. The relation*

$$\rho_l(P, \rho, C = C_{eq}) = \frac{1}{\tau_l^s(P)}$$

implies that:

$$h_{HEM}(P, \rho) = h_{HRM}(P, \rho, C = C_{eq})$$

Remark 13 *The relaxation source term (4.9) of the HRM model can now be written:*

$$\Gamma = (1 - C) (C_{eq}(P, \rho) - C) \frac{G_2(P, \rho)}{\tau_0} \quad (4.17)$$

Then $C = C_{eq}(P, \rho)$ is a curve for the equilibrium $\Gamma = 0$.

4.3.2 Hyperbolicity

In order to study the hyperbolicity of the HEM model, we focus on the convective part of (4.14). Then the non-conservative equations on ρ , U and P are:

$$\partial_t \begin{pmatrix} \rho \\ U \\ P \end{pmatrix} + \begin{pmatrix} U & \rho & 0 \\ 0 & U & \tau \\ 0 & \hat{\gamma}_{HEM}P & U \end{pmatrix} \partial_x \begin{pmatrix} \rho \\ U \\ P \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad (4.18)$$

with:

$$\hat{\gamma}_{HEM}P = (\partial_P(e_{HEM}))^{-1} \left(\frac{P}{\rho} - \rho \partial_\rho(e_{HEM}) \right)$$

The eigenvalues and eigenvectors of the matrix of the system (4.18) can be found in the appendix 1. It appears that the system is hyperbolic if and only if $\hat{\gamma}_{HEM}P > 0$. We classically define the sound velocity a_{HEM} by:

$$\rho a_{HEM}^2 \stackrel{def}{=} \hat{\gamma}_{HEM}P \quad (4.19)$$

Since the derivatives of e_{HEM} are not defined in the whole domain D , γ_{HEM} is only defined inside the subdomains D_l and $D_{2\Phi}$.

The sound speed then reads:

- In the pure liquid domain: $a_{HEM} = \sqrt{\gamma_l P \tau} = \sqrt{\frac{\delta_l}{\delta_l - 1} P \tau} \quad \forall (\tau, P) \in \overset{\circ}{D}_l$
- In the two-phase domain the formulas are cumbersome and no sufficient condition clearly appears to ensure the positivity of a_{HEM}^2 . For all couple (τ, P) in $\overset{\circ}{D}_{2\Phi}$, we have:

$$\rho a_{HEM}^2 = \frac{\left(\frac{P}{\rho} - \rho \partial_\rho(e_{HEM}) \right)}{\partial_P(e_{HEM})} \quad (4.20)$$

with:

$$\left(\frac{P}{\rho} - \rho \partial_\rho (e_{HEM}) \right) = \rho \partial_\rho (C_{eq}) (h_v^s - h_l^s)$$

$$\partial_P (e_{HEM}) = -\tau + \partial_P (C_{eq}) (h_l^s - h_v^s) + C_{eq} \frac{d}{dP} h_l^s + (1 - C_{eq}) \frac{d}{dP} h_v^s$$

Nonetheless it can be shown that, with our choices for the saturation curves and for the chosen perfect gas coefficients, $\frac{P}{\rho} - \rho \partial_\rho (e_{HEM})$ and $\partial_P (e_{HEM})$ remain positive inside the two-phase domain $D_{2\Phi}$.

Finally, the HEM model is hyperbolic inside the pure liquid domain and inside the two-phase domain.

4.3.3 Preservation of physically relevant values and entropy inequality for the HEM model

We start again with the non-conservative form (4.18) of the HEM model. Defining:

$$\eta_{HEM} = -\rho \ln(S_{HEM})$$

$$F_\eta^{HEM} = U \eta_{HEM}$$

where the entropy S_{HEM} agrees with:

$$\hat{\gamma}_{HEM} P \partial_P (S_{HEM}) + \rho \partial_\rho (S_{HEM}) = 0 \quad (4.21)$$

and using the classical argument of the vanishing viscosity enables to retrieve the entropy inequality:

$$\partial_t (\eta_{HEM}) + \partial_x (F_\eta^{HEM}) \leq 0 \quad (4.22)$$

Moreover, the HEM model maintains positive values of pressure and density.

4.4 A method to couple HEM and HRM models

We want to couple an "HEM" code and an "HRM" code through a fictitious interface $x = 0$.

One of the main difficulties which arise when one aims at coupling the HRM and HEM models is due to the fact that the liquid mass fraction C is governed by a PDE in the HRM, and issues from a local constraint $C = C_{eq}(P, \rho)$ in the HEM model. We propose to couple both models using a "father interface model" with an instantaneous relaxation process at the interface. In [52], a similar approach was used to couple a one dimensional code and a two dimensional code, following ideas from [44]. In the present approach, we rather choose to proceed as in [4, 6]. The main advantage is that one can get rid of the possible resonance phenomenon.

4.4.1 The interface model

We first rewrite the HEM set of equations. This is achieved introducing a PDE with a source term containing an instantaneous relaxation term:

$$\partial_t (\rho C) + \partial_x (\rho U C) = \mu \rho (C_{eq}(P, \rho) - C) \quad \text{with} \quad \mu = +\infty$$

The set of equations for the HEM model thus writes:

$$\begin{cases} \partial_t (\rho C) + \partial_x (\rho U C) = \mu \rho (C_{eq}(P, \rho) - C) \\ \partial_t (\rho) + \partial_x (\rho U) = 0 \\ \partial_t (\rho U) + \partial_x (\rho U^2 + P) = 0 \\ \partial_t (\rho E) + \partial_x (U(\rho E + P)) = 0 \end{cases} \quad (4.23)$$

with the parameter $\mu = +\infty$.

We may now introduce the "father model". For that purpose we define a new variable $Y(x, t)$ depending on time and space. At the time $t = 0$ we initialize $Y_0(x) = Y(x, 0)$ such that $Y_0(x) = 1$ if x is in the HRM domain and $Y_0(x) = 0$ if x is in the HEM domain. The "father model" is governed by the following set of equations:

$$\begin{cases} \partial_t (\rho C) + \partial_x (\rho C U) = \rho T \\ \partial_t (\rho) + \partial_x (\rho U) = 0 \\ \partial_t (\rho U) + \partial_x (\rho U^2 + P) = 0 \\ \partial_t (\rho E) + \partial_x (U(\rho E + P)) = 0 \\ \partial_t (\rho Y) + \partial_x (\rho U Y) = \lambda \rho (Y_0 - Y) \end{cases} \quad (4.24)$$

with:

$$E = Y e_{HRM}(P, \rho, C) + (1 - Y) e_{HEM}(P, \rho) + \frac{u^2}{2}$$

and

$$T = Y \Gamma + (1 - Y) \mu (C_{eq} - C)$$

The variable Y is usually called the "color variable". In the following the parameters λ and μ will formally be set to $+\infty$ (instantaneous relaxation).

We may define a sound speed a for this interface model, which reads:

$$a^2 = \frac{a_{HRM}^2 Y \partial_P (e_{HRM}) + a_{HEM}^2 (1 - Y) \partial_P (e_{HEM})}{Y \partial_P (e_{HRM}) + (1 - Y) \partial_P (e_{HEM})} \quad (4.25)$$

The system (4.24) is hyperbolic if and only if $a^2 > 0$. We know from the study of the HEM and HRM models that $\partial_P (e_{HRM})$, $\partial_P (e_{HEM})$, a_{HRM}^2 and a_{HEM}^2 are positive if (C, ρ, P) is in the domain $D_{HRM} \cap (D_{2\Phi} \cup D_l)$. Furthermore, the system (4.24) ensures that if Y_0 is in $[0, 1]$, Y remains in $[0, 1]$. Hence a^2 is positive and the system (4.24) is hyperbolic if $(C, \rho, P) \in D_{HRM} \cap (D_{2\Phi} \cup D_l)$.

4.4.2 Numerical scheme

All methods described herein rely on the Finite Volume method ([27, 37]) . We restrict here to the so-called "first-order" schemes. We will apply for the approximate Godunov scheme VFRoe-ncv using the non conservative variable (ρ, U, P) for the HEM system and (ρ, U, P, C) for the HRM system (see[16, 31] for details on these approximate Godunov schemes). The coupling interface model which has been introduced above will be used to compute "fluxes" at the interface between the two domains.

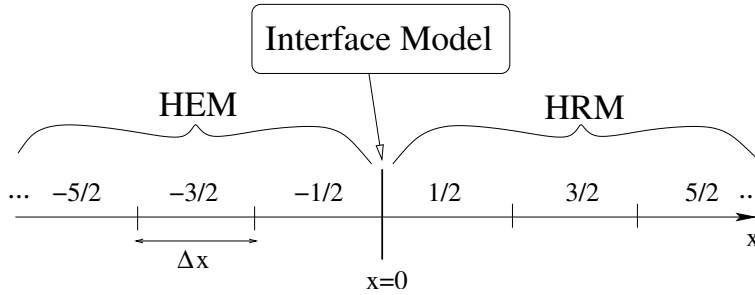


FIG. 4.1 – Notations and models.

Let us introduce a fixed uniform mesh space Δx and a time step Δt in agreement with a CFL condition. We set for all integers j and n ,

$$x_{j+1/2} = (j + \frac{1}{2})\Delta x, \quad x_j = j\Delta x, \quad t^n = n\Delta t$$

The cell $j + 1/2$ is delimited by the interface j located in x_j and the interface $j + 1$ located in x_{j+1} , and its center is denoted by $x_{j+1/2}$. The interface $j = 0$ is the coupling interface. The variable $W_{j+1/2}^n$ stands for the variable W at the time t^n in the cell $j + 1/2$. The HEM domain (and the HRM domain respectively) is composed of all the cells $j + 1/2 < 0$ (respectively of all the cells $j + 1/2 > 0$, see figure (4.1)). The conservative variables will be denoted by $W_{HEM} = (\rho, \rho U, \rho E_{HEM})^\top$ in the HEM domain, $W_{HRM} = (\rho C, \rho, \rho U, \rho E_{HRM})^\top$ in the HRM domain and by $W_{INT} = (\rho C, \rho, \rho U, \rho E, \rho Y)^\top$ for the interface model.

We assume that $Y_{j+1/2}^n = 0$ for all $j + 1/2 \leq 0$ and $Y_{j+1/2}^n = 1$ for all $j + 1/2 \geq 0$ at a discrete time t^n . The numerical scheme which is used to compute the variable at time step $t^{n+1} = t^n + \Delta t$ contains three steps:

- 1) A convection step, $t^n \rightarrow t^{\tilde{n}}$.
- 2) An instantaneous relaxation on Y , $t^{\tilde{n}} \rightarrow t^{\hat{n}}$.
- 3) A finite relaxation step, $t^{\hat{n}} \rightarrow t^{n+1}$.

The convection step, $t^n \rightarrow t^{\tilde{n}}$

This step of the scheme does not take into account the different source terms. The fluxes are computed at each interface j .

- (i) For all interface $j \leq -1$ (HEM domain) we apply the VFRoe-ncv scheme using the variable $(\rho, U, P)^\top$ on the convective part of the system (4.14). The flux is denoted $F_{HEM,j}^n$.
- (ii) For all interface $j \geq 1$ (HRM domain) we apply VFRoe-ncv scheme using the variable $(C, \rho, U, P)^\top$ on the convective part of the system (4.1). The flux is denoted $F_{HRM,j}^n$.
- (iii) At $j = 0$ (the coupling interface) the flux is built with a modified VFRoe-ncv scheme which uses the variable $(C, \rho, U, P, Y)^\top$ in order to compute approximate interface states in the solution of the one-dimensional Riemann problem associated with the system (4.24). The left state in the initial condition of the Riemann problem is

$$((\rho C_{eq}(P, \rho))_{-1/2}^n, \rho_{-1/2}^n, (\rho U)_{-1/2}^n, (\rho E_{HEM})_{-1/2}^n, (\rho Y)_{-1/2}^n)^\top$$

and the right state in the initial condition is

$$((\rho C)_{1/2}^n, \rho_{1/2}^n, (\rho U)_{1/2}^n, (\rho E_{HRM})_{1/2}^n, (\rho Y)_{1/2}^n)^\top$$

The flux is denoted $F_{INT,j}^n$. Details on the computation of $F_{INT,j}^n$ are given in Appendix 1.

Once the fluxes have been computed for all interfaces, the value of the cell is updated using the formula:

- If $j + 1/2 \leq -3/2$

$$W_{HEM,j+1/2}^{\tilde{n}} - W_{HEM,j+1/2}^n + \frac{\Delta t}{\Delta x} (F_{HEM,j}^n - F_{HEM,j-1}^n) = 0$$

- If $j + 1/2 \geq 3/2$

$$W_{HRM,j+1/2}^{\tilde{n}} - W_{HRM,j+1/2}^n + \frac{\Delta t}{\Delta x} (F_{HRM,j}^n - F_{HRM,j-1}^n) = 0$$

- If $j + 1/2 = -1/2$

$$\left(\begin{array}{c} W_{HEM} \\ \rho Y \end{array} \right)_{-1/2}^{\tilde{n}} - \left(\begin{array}{c} W_{HEM} \\ \rho Y \end{array} \right)_{-1/2}^n + \frac{\Delta t}{\Delta x} \left((F_{2-5})_{INT}^n - \left(\begin{array}{c} F_{HEM,-1}^n \\ (\rho U Y)_{HEM,-1}^n \end{array} \right) \right) = 0$$

The flux $(F_{2-5})_{INT}^n$ is composed of the second, third, fourth and fifth components of F_{INT}^n

- If $j + 1/2 = 1/2$

$$\left(\begin{array}{c} W_{HRM} \\ \rho Y \end{array} \right)_{1/2}^{\tilde{n}} - \left(\begin{array}{c} W_{HRM} \\ \rho Y \end{array} \right)_{1/2}^n + \frac{\Delta t}{\Delta x} \left(\left(\begin{array}{c} F_{HRM,1}^n \\ (\rho U Y)_{HRM,1}^n \end{array} \right) - F_{INT}^n \right) = 0$$

An important point to be quoted is that: $Y_{j+1/2}^{\tilde{n}} = Y_{j+1/2}^n$ in all the cells, except in the cell $j = 1/2$ if $U_{INT}^n > 0$ and in the cell $j = -1/2$ if $U_{INT}^n < 0$.

Instantaneous relaxation step, $t^{\tilde{n}} \rightarrow t^{\hat{n}}$

For this step we consider the ODE system on the whole domain ($x \in \mathbb{R}$):

$$\left\{ \begin{array}{l} \partial_t (\rho C) = 0 \\ \partial_t (\rho) = 0 \\ \partial_t (\rho U) = 0 \\ \partial_t (\rho E) = 0 \\ \partial_t (\rho Y) = \lambda \rho (Y_0 - Y) \text{ with } \lambda = +\infty \end{array} \right. \iff \left\{ \begin{array}{l} \partial_t (\rho C) = 0 \\ \partial_t (\rho) = 0 \\ \partial_t (\rho U) = 0 \\ \partial_t (\rho E) = 0 \\ Y = Y_0 \end{array} \right. \quad (4.26)$$

This can be rewritten in terms of discrete variables (for all k) as:

$$\left\{ \begin{array}{l} (\rho C)_k^{\hat{n}} = (\rho C)_k^{\tilde{n}} \\ \rho_k^{\hat{n}} = \rho_k^{\tilde{n}} \\ (\rho U)_k^{\hat{n}} = (\rho U)_k^{\tilde{n}} \\ (\rho E)_k^{\hat{n}} = (\rho E)_k^{\tilde{n}} \\ Y_k^{\hat{n}} = Y_k^0 \end{array} \right. \text{ and thus } \left\{ \begin{array}{l} C_k^{\hat{n}} = C_k^{\tilde{n}} \\ \rho_k^{\hat{n}} = \rho_k^{\tilde{n}} \\ U_k^{\hat{n}} = U_k^{\tilde{n}} \\ e_k^{\hat{n}} = e_k^{\tilde{n}} \\ Y_k^{\hat{n}} = Y_k^0 \end{array} \right. \quad (4.27)$$

This step is totally transparent with respect to physical conservative variables. Let us call k the cell $j + 1/2$ for which $Y_{j+1/2}^{\tilde{n}} \neq Y_{j+1/2}^n$, for all the other cells we have $Y_{j+1/2}^{\tilde{n}} = Y_{j+1/2}^0$. The fourth equation of (4.27) implies that the pressure changes in the cell k during the current step. Indeed equations (4.27) imply:

$$e(P_k^{\hat{n}}, \rho_k^{\tilde{n}}, C_k^{\tilde{n}}, Y_k^{\hat{n}}) = e(P_k^{\tilde{n}}, \rho_k^{\tilde{n}}, C_k^{\tilde{n}}, Y_k^{\tilde{n}}) \quad (4.28)$$

Thus $Y_k^{\hat{n}} \neq Y_k^{\tilde{n}}$ implies that $P_k^{\hat{n}} \neq P_k^{\tilde{n}}$.

The finite time relaxation step, $t^{\hat{n}} \rightarrow t^{n+1}$

In this final step we compute the source term T setting $\mu = +\infty$. It only remains to solve the ODE system for $x > 0$:

$$\left\{ \begin{array}{l} \partial_t (\rho C) = \rho \Gamma \\ \partial_t (\rho) = 0 \\ \partial_t (\rho U) = 0 \\ \partial_t (\rho E) = 0 \end{array} \right. \quad (4.29)$$

in the HRM domain. In terms of the non-conservative variables (C, ρ, U, P) and regular solutions, (4.29) is equivalent to:

$$\left\{ \begin{array}{l} \partial_t (C) = \Gamma \\ \partial_t (\rho) = 0 \\ \partial_t (U) = 0 \\ \partial_t (P) = -(\partial_P (e_{HRM}))^{-1} \partial_C (e_{HRM}) \Gamma \end{array} \right. \quad (4.30)$$

Remark 14 *Since $\partial_P (e_{HRM}) > 0$ and $\partial_C (e_{HRM}) > 0$, the time derivatives of the liquid mass fraction and of the pressure have an opposite sign.*

The time discretization of the system (4.30) is:

$$\left\{ \begin{array}{l} (\rho C)^{n+1} = \rho^{\hat{n}} C^{n+1} \\ \rho^{n+1} = \rho^{\hat{n}} \\ (\rho U)^{n+1} = (\rho U)^{\hat{n}} \\ (\rho E)^{n+1} = \rho^{\hat{n}} \left(e_{HRM}(P^{n+1}, \rho^{\hat{n}}, C^{n+1}, Y^{\hat{n}}) + \frac{(U^{\hat{n}})^2}{2} \right) \\ (\rho Y)^{n+1} = (\rho Y)^{\hat{n}} \end{array} \right. \quad (4.31)$$

The details of the computation of C^{n+1} and P^{n+1} can be found in Appendix 2.

4.4.3 Remarks

- The convection step (thanks to the VFRoe-ncv scheme and the respect of the CFL condition) and the instantaneous relaxation step maintain the discrete liquid mass fraction $C^{\hat{n}}$ in $[0,1]$. Moreover, if the discrete values of the equilibrium liquid mass fraction C_{eq} remain in $[0,1]$ during all the finite time relaxation computation, C^{n+1} will remain in $[0,1]$ (see Appendix 2).
- The introduction of the fictive variable Y does not lead to any modification of the left and right codes, except for boundary conditions of course.

4.5 Numerical results

Many test cases involving single waves, and in particular contact waves enable to check that numerical methods used within each code are well-suited. More precisely, the exact analytical form of the internal energy, for both the HEM and the HRM models, is such that the approximate Godunov scheme VFROE-ncv (using variables U, P, ρ and U, P, ρ, C for HEM and HRM models respectively) perfectly preserves these pure contact waves on coarse and fine meshes (see[30]) . This is still true for the coupled HEM/HRM model, for similar reasons (see Appendix 3).

The different parameters will be set as follows:

$$P_{MIN} = 0.1 \cdot 10^5 \text{ Pa} \quad \text{and} \quad P_{MAX} = 200 \cdot 10^5 \text{ Pa}$$

$$\gamma_l = 1.001 \quad \text{and} \quad \gamma_v = 1.4$$

The exact form of the saturation curves is obtained using the following numerical values:

$$h_l^s = A_l P + B_l \quad h_v^s = A_v P + B_v$$

with the coefficients:

$$A_l = 8.18 \cdot 10^{-2} \quad B_l = 1.91 \cdot 10^5 \quad A_v = -8.32 \cdot 10^{-3} \quad B_v = 2.58 \cdot 10^6 \quad (4.32)$$

The whole data correspond to nuclear cooling condition.

We successively consider two different test cases which correspond to:

- the computation of Riemann problems including shock waves, contact waves and rarefaction waves,
- a schematic computation of the flow in the coolant circuit of a nuclear power plant.

4.5.1 Riemann problems

We consider in this section a computational domain: $x \in [-1,1]$ which is discretized using a uniform mesh. We will compare for different mesh sizes, the results obtained with:

- The Homogeneous Equilibrium Model over the whole computational domain,
- The Homogeneous Relaxation Model over the whole computational domain,
- The coupling configuration in which HEM is used for $x < 0$, HRM is used for $x > 0$, and the coupling technique described in section IV is applied for $x = 0$.

Hence, we will be able to compare the results of the coupled case with those obtained with a "reference solution", which will correspond with either the HEM results (or the HRM results) computed on a very fine mesh.

We focus here on test cases that are based on Riemann problems, where the initial discontinuity will be located either in the HEM code ($x = -0.25$), or in the HRM code ($x = +0.25$), as described in figures (4.2) and (4.3).

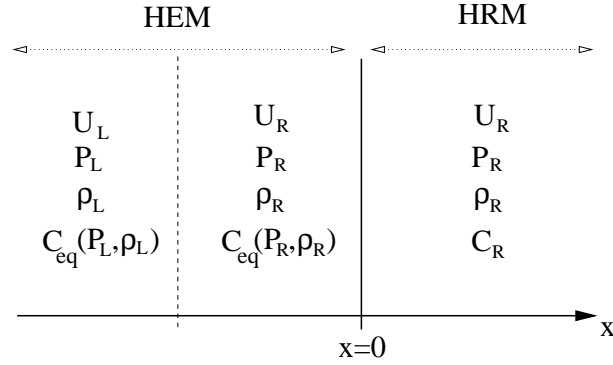


FIG. 4.2 – First configuration for initial data, the initial discontinuity is in the HEM domain

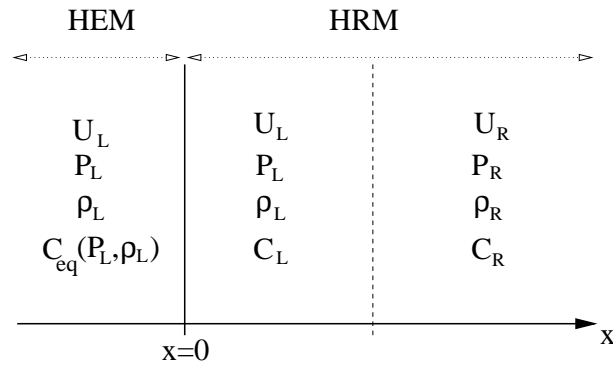


FIG. 4.3 – Second configuration for initial data, the initial discontinuity is in the HRM domain

The main goal here is to observe the behavior of transmitted and reflected waves through the interface $x = 0$, and the numerical pollution due to the coupling scheme.

We emphasize that :

- Three different meshes will be used. An "industrial" mesh with 100 cells (fifty cells within each code), a medium sized mesh with 500 cells, and a fine mesh including 10000 cells that will provide "almost converged" solutions.
- Rarefaction waves will be investigated, with special emphasis on the reflected and transmitted waves through the coupling interface. The counterpart including the propagation of shock waves through the coupling interface is reported in[55] . Rarefaction waves are of special interest in the nuclear framework, since the smooth solution corresponds to the Loss Of Coolant Accident (LOCA).
- The time relaxation parameter $\tau_0^2 = 10^{-3}$ will be used. (similar tests with a different time scale $\tau_0^1 = 1$ are reported in[55]) . In fact the τ_0 the smaller, the similarity in the behaviour of the HRM and the HEM models the better.

In each case, two series of results are shown:

- We have gathered computations for the HEM model, HRM model and the HEM/HRM simulation on coarse meshes in order to highlight the influence of the coupling in industrial configuration (see figures (4.4) and (4.6)).

- Fine mesh computations for the HEM model and HRM model have been performed. They are plotted together with the results of the HEM/HRM simulation for all the meshes on the figure (4.5) and (4.7).

Hence, results include:

- a computation of the HEM model on the whole domain, using a mesh with 100 cells (circles);
- a computation of the HRM model on the whole domain, using a mesh with 100 cells (triangles);
- a computation of the coupled case HEM ($x < 0$)-HRM ($x > 0$), using a mesh with 100 cells (plain line).

A comparison is also made between results for:

- the "converged" HEM model on the whole domain, using a mesh with 10000 cells (circles);
- the "converged" HRM model on the whole domain, using a mesh with 10000 cells (triangles);
- the "converged" coupled case HEM ($x < 0$)-HRM ($x > 0$), using a mesh with 10000 cells (plain line);
- the coupled case HEM ($x < 0$)-HRM ($x > 0$), using coarse meshes with 100, 500 cells (dotted line, dashed line).

In each case we plot numerical results before the contact discontinuity hits the coupling interface $x = 0$. The time step agrees with the classical CFL condition. The implicit treatment of source terms implies no additional constraint. Numerical experiments include:

- a rarefaction wave travelling from the HEM code to the HRM code;
- a rarefaction wave travelling from the HRM code to the HEM code

The dual case of shock waves is investigated in[55], and the last industrial test case contains such a configuration.

A rarefaction wave traveling from HEM domain to HRM domain

Initial conditions are:

domain :	HEM	HEM	HRM
U	0	0	0
P	158e5	160e5	160e5
ρ	990	1000	1000
C	none	none	0.979212418
C_{eq}	0.979261526	0.979212418	0.979212418

The initial discontinuity has been set at $x = -0.25$, that is inside the HEM domain. A rarefaction wave travels towards the right and goes through the coupling interface ($x = 0$), a shock wave travels to the left, and is followed by a left-going contact discontinuity. Results have been plotted at time $t = 0.025$. We notice that for the HEM computation, the whole right-going rarefaction wave has passed the coupling interface at that time.

Associated results for the sole HRM model are indeed rather close to the solutions computed with the sole HEM model. Turning then to the coupled situation, we note that the rarefaction wave coming from the HEM code does not introduce too much pollution when passing through the coupling interface, though one can notice a sharp behaviour of the pressure field around $x = 0$, when the mesh is too coarse (100 cells, corresponding to the plain line on figure (4.4)). In the coupled computation, the approximate solution in the HRM domain (respectively in the HEM domain) tends to stick immediately to the pure HRM solution (respectively to the pure HEM solution).

Another point which seems worth being underlined is that the pollution around the coupling interface, which looks almost steady in some cases (see figure (4.4) and (4.5) for instance) tends to decrease and also clearly moves away from this interface when the mesh is refined. This clearly appears when looking at the dashed line on figure (4.4) and also on figure (4.5).

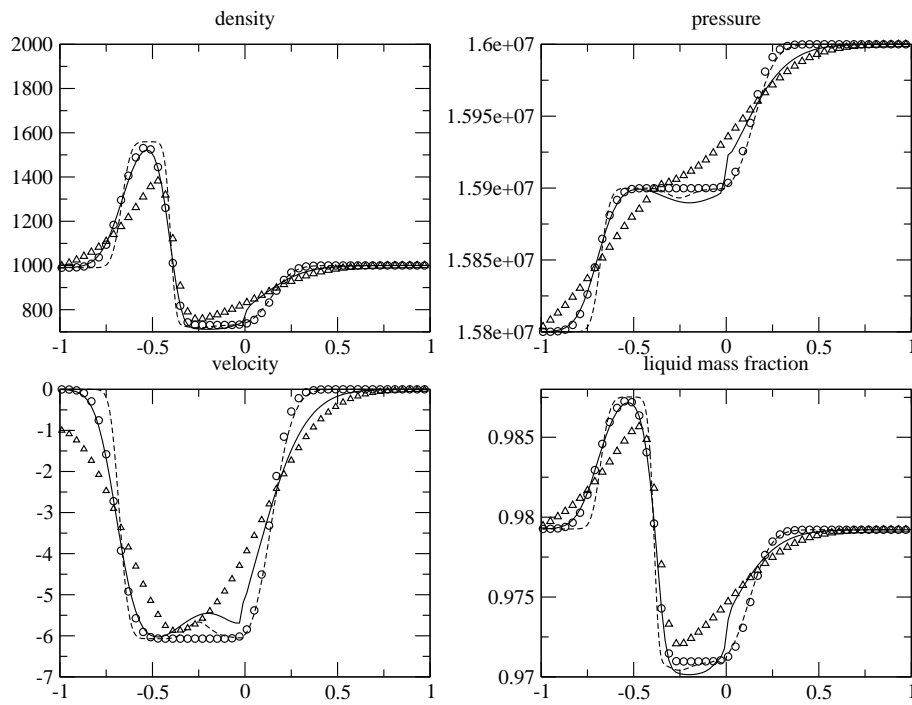


FIG. 4.4 - Constant time scale τ_0^2 . Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, dashed line=HEM/HRM 500 cells.

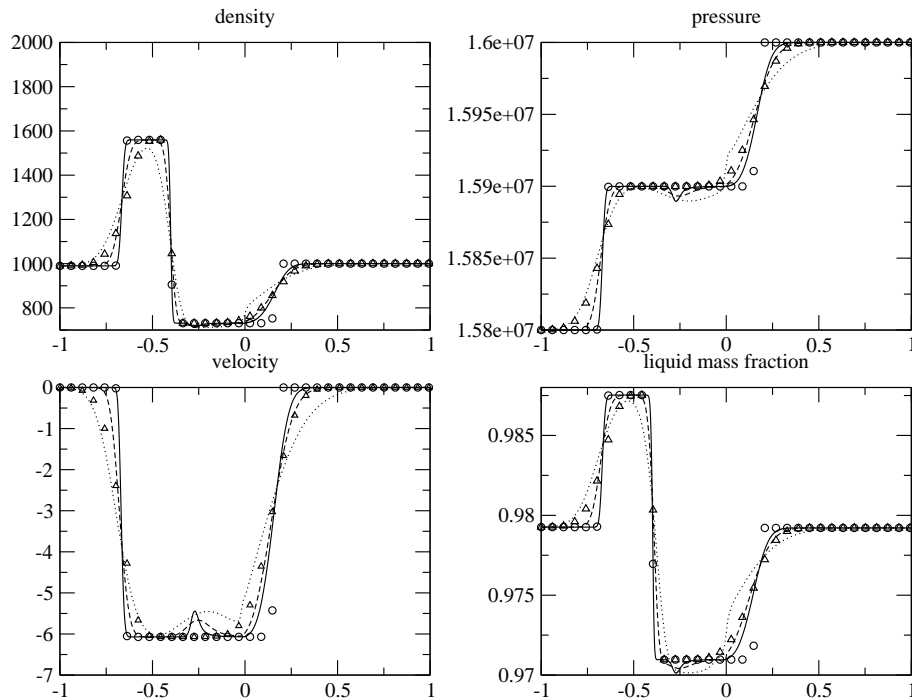


FIG. 4.5 - Constant time scale τ_0^2 . Circles=HEM 10000 cells, triangles=HRM 10000 cells, line=HEM/HRM 10000 cells, dashed line=HEM/HRM 500 cells, dot line=HEM/HRM 100 cells.

A rarefaction wave traveling from HRM domain to HEM domain

Initial conditions are now the following:

domain :	HEM	HRM	HRM
U	0	0	0
P	160e5	160e5	158e5
ρ	1000	1000	990
C	none	0.979212418	0.979261526
C_{eq}	0.979212418	0.979212418	0.979261526

The initial discontinuity is now in the HRM domain, and is located at $x = 0.25$. A rarefaction wave travels to the left and goes through the coupling interface ($x = 0$). Meanwhile a shock wave travels to the right boundary, and is followed by a contact discontinuity that travels towards the right. Results are still plotted at time $t = 0.025$. At that time, the left-going rarefaction wave is entirely in the HEM domain in the sole HEM computation.

Remarks pertaining to the previous test case still hold. The mesh refinement helps much to improve the accuracy of the approximate solution in each subdomain. In the coupled simulation, the approximate solution occurs to be much more monotone around the coupling interface when the mesh is refined (see figure (4.7)).

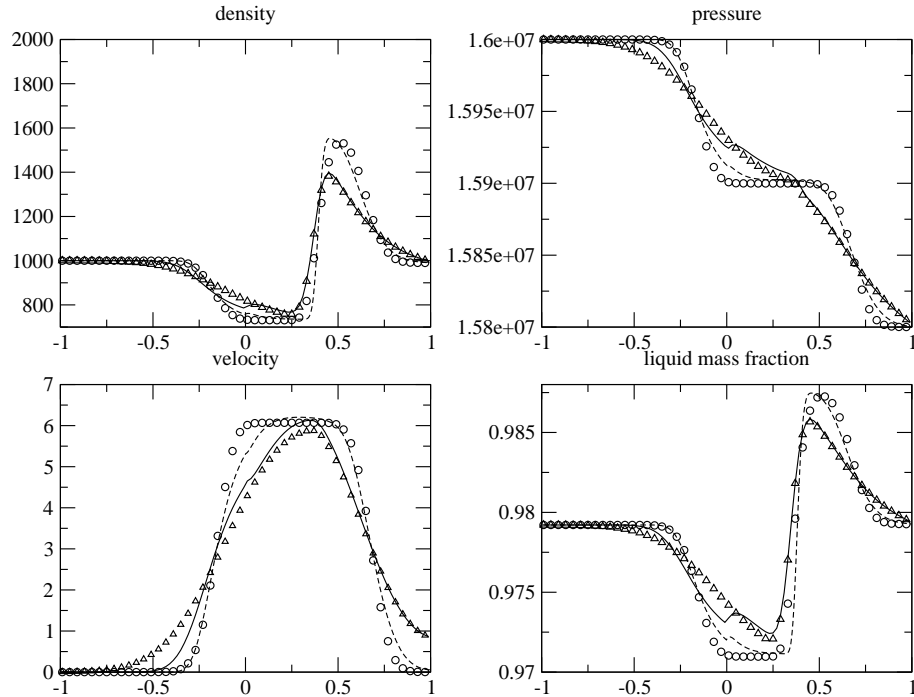


FIG. 4.6 – Constant time scale τ_0^2 . Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, dashed line=HEM/HRM 500 cells.

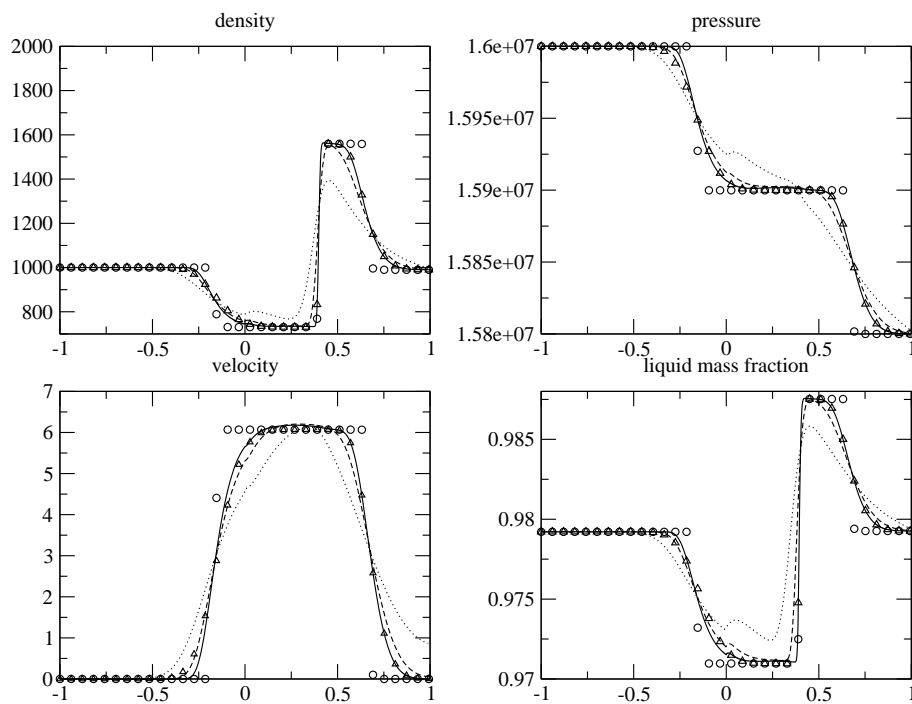


FIG. 4.7 – Constant time scale τ_0^2 . Circles=HEM 10000 cells, triangles=HRM 10000 cells, line=HEM/HRM 10000 cells, dashed line=HEM/HRM 500 cells, dot line=HEM/HRM 100 cells.

4.5.2 A test case in a nuclear power plant

The next test case corresponds to the schematic one dimensional flow in a nuclear power plant. The length of the pipes is 80 m. It includes a part of the coolant circuit containing the core on the left side of the coupling interface (i.e. $-40 < x < 0$) where the governing set of equations is the HEM model. The core is located in the interval $[-22, -18]$. The total length of the core is the true core length (buoyancy effects can be neglected). The core section is equal to 3.5 m^2 . The HRM model is used on the right side of the coupling interface (i.e. $0 < x < 40$). Before the beginning of the computation, the velocity, density and pressure profiles are uniform and equal to: $U = 10 \text{ m.s}^{-1}$, $\rho = 700 \text{ kgm}^{-3}$, $P = 150 \cdot 10^5 \text{ Pa}$; moreover $C = C_{eq}(P, \rho)$ in the HRM part of the coolant circuit. The fluid is not heated before the beginning of the computation, and the core is suddenly plugged in the coolant circuit at that time. Then the heat source $\Phi(x, t > 0)$ is null outside the core. Within the core region, the heat source is uniform and such that :

$$\int_{x=-22}^{x=-18} \Phi(x, t > 0) dx = \Phi_0 = 300 \cdot 10^6 \text{ W}$$

In this particular test case the constants A_v , B_v , A_l , and B_l have been estimated with $P_{MIN} = 140 \cdot 10^5 \text{ Pa}$ and $P_{MAX} = 160 \cdot 10^5 \text{ Pa}$ using the Thetis software[65] . The uniform mesh contains 500 nodes. The governing set of equations in the left part is the set of equations of the HEM model (4.14) with an equation for the total energy which takes into account the heat source:

$$\partial_t(\rho E) + \partial_x(U(\rho E + P)) = \Phi(x)$$

Results have been plotted at four distinct instants.

- At $t = T_1$, the right-going shock wave, which is coming from the right side of the core, and which is due to the sudden heating in the core region, has not hit the coupling interface yet (dashed line on figure (4.8)).
- At $t = T_2$, the same right-going shock wave has already moved through the coupling interface (plain line on figure (4.8)). One can easily observe at $t = T_2$ the reflected wave in the interval $[-10, 0]$, either focusing on the pressure profile, the density profile or the velocity profile. The amplitude of this reflected wave is small compared with the one of the associated shock wave.
- At $t = T_3$, the right-going contact wave has still not passed the coupling interface (dashed line on figure (4.9)). This contact wave is of course characterized by locally uniform pressure and velocity profiles. At that time, the right going shock wave has not reached the right exit. The behaviour of the coupling interface seems almost perfect, which is in agreement with test cases involving a contact wave travelling from the HEM domain towards the HRM domain (see[55]) .
- At $t = T_4$, the contact wave is on the right side of the coupling interface ($x = 0$) (plain line on figure (4.9)). Once again, everything is correct around the coupling interface ($x = 0$). At that time $t = T_4$, the right-going shock wave has gone outside the computational domain. One can notice the influence of the right exit boundary which generates a reflected wave in the computational domain. This is due to the fact that crude "Neumann-type" boundary conditions have been imposed in this test case.

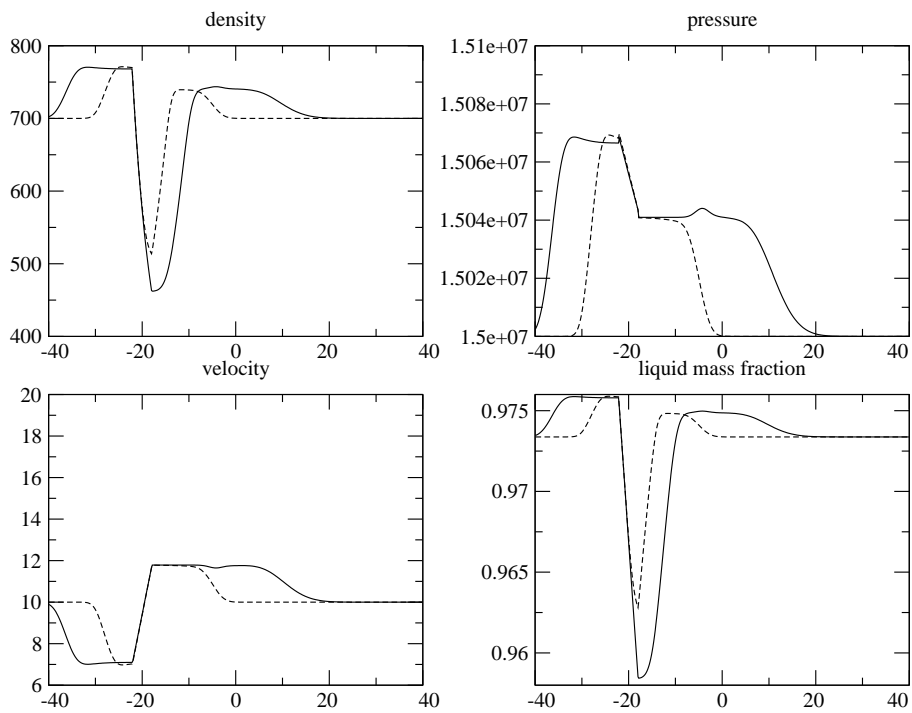


FIG. 4.8 – Interaction of the shock wave with the coupling interface. Dashed line ($t = T_1$): the shock wave has not hit the coupling interface. Plain line ($t = T_2$): the shock wave has passed the coupling interface.

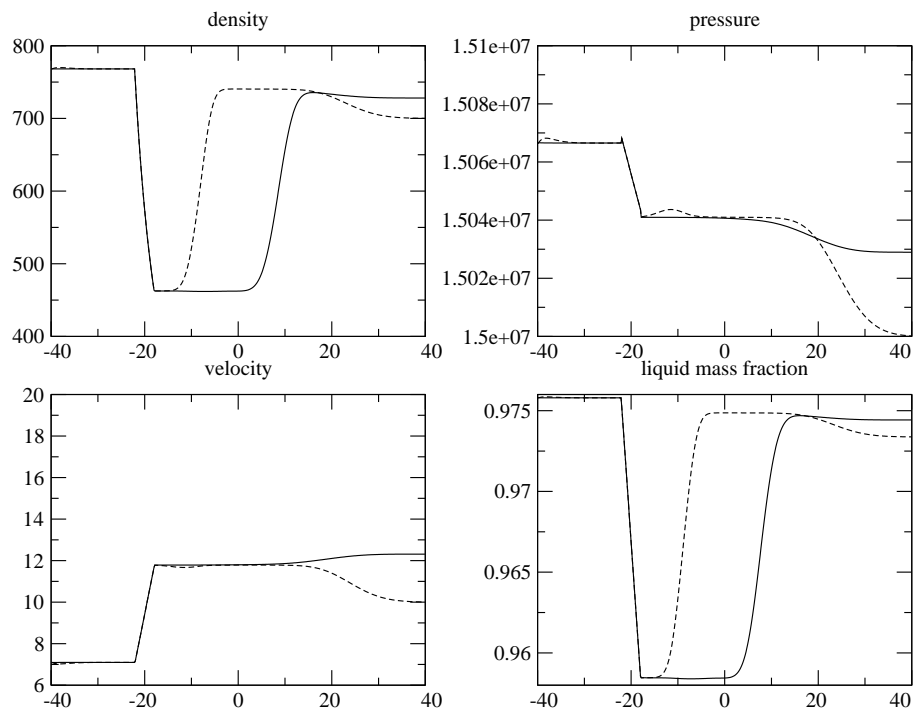


FIG. 4.9 – Interaction of the contact wave with the coupling interface. Dashed line ($t = T_3$): the contact wave has not hit the coupling interface. Plain line ($t = T_4$): the contact wave has passed the coupling interface.

4.6 Conclusion

This work (one should also read[7] for a companion work on that topic) is a first attempt to couple two different codes that provide numerical approximations of HEM and HRM models. These two models have been recalled, together with closure laws including EOS. We have chosen here a coupling method inspired by[4] , which is essentially different from the one that has been investigated in[52] . Its simplicity is appealing, and it enables to circumvent the tough problem of resonance at the coupling interface.

Some properties of both models, and the main properties of algorithms involved in sole codes have been given or recalled. Some properties of the coupling method have also been detailed. One may say that the whole approach is rather efficient, and we would like to emphasize the rather nice behaviour of the coupled approach when contact waves travel through codes. The reader must be aware that some numerical properties deeply rely on the approximate Godunov schemes ([30]) which are used in sole codes. The coupling approach preserves the conservative form of mass, momentum and total energy equations. It also seems worth emphasizing the following features:

- If one restricts to coarse meshes, which is obviously the correct framework for industrial applications, it also occurs that incompatibilities between formulations may be smoothed with this formulation, owing to the dissipative nature of upwinding techniques which have been applied inside codes and at the coupling interface. This is indeed flagrant if one focuses on relaxation time scales. Some of the numerical results presented in[55] confirm that one can cope with decorrelated signals (owing to very large relaxation times in the HRM model) on coarse meshes, but that this no longer holds when refining the mesh. This is much in favour of the coupling approach, since it may be understood as a tool which automatically checks whether both models on each side of the interface are in agreement or not.
- A much deeper insight on thermodynamics is actually deserved. Special emphasis should be given on the respective saturation curves for the liquid phase and the vapour phase. Some comments may be picked up in this manuscript, which might perhaps help improving the global formulation (see Appendix 4). We suggest that it would be a better idea to use the same thermodynamic tables in both codes. Thus, it would be interesting to examine whether the formalism introduced in [47] might help improving the whole thermodynamical representation.
- Another problem concerns the formulation of mass transfer terms. The one which has been considered here relies on: $\Gamma = K(1 - C)C(h_l^s(P) - h_l(P, \rho_l))$. Alternative formulations that preserve entropic properties should actually be preferred (see for instance[17, 57, 19]).

Acknowledgements

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4.7 Appendix 1: The VFRoe-ncv scheme and its modified version

4.7.1 The VFRoe-ncv scheme

We define herein the basic first order approximate Godunov scheme and restrict to regular meshes of size Δx such that: $\Delta x = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$, $i \in \mathbb{Z}$. We denote Δt the time step, where $\Delta t = t^{n+1} - t^n$, $n \in \mathbb{N}$. In order to approximate solutions of the exact solution $W \in \mathbb{R}^p$ of the conservative hyperbolic system:

$$\begin{cases} \partial_t(W) + \partial_x(F(W)) = 0 \\ W(x,0) = W_0(x) \end{cases}$$

with $F(W)$ in \mathbb{R}^p . Let W_i^n be the approximate value of $\frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} W(x,t^n) dx$. Integrating over $[x_{i-\frac{1}{2}}; x_{i+\frac{1}{2}}] \times [t^n; t^{n+1}]$ provides:

$$W_i^{n+1} = W_i^n - \frac{\Delta t}{\Delta x} (\phi_{i+\frac{1}{2}}^n - \phi_{i-\frac{1}{2}}^n)$$

The numerical flux $\phi_{i+\frac{1}{2}}^n$ through the interface $\{x_{i+\frac{1}{2}}\} \times [t^n; t^{n+1}]$ is defined below. The time step must agree with a CFL condition detailed below. The flux $\phi_{i+\frac{1}{2}}^n$ depends on W_i^n and W_{i+1}^n when restricting to first order schemes. The approximate Godunov flux $\phi(W_L, W_R)$ is obtained by solving exactly the following linear 1D Riemann problem:

$$\begin{cases} \partial_t(Y) + B(\hat{Y})\partial_x(Y) = 0 \\ Y(x,0) = \begin{cases} Y_L & \text{if } x < 0 \\ Y_R & \text{otherwise} \end{cases} \end{cases} \quad (4.33)$$

and initial condition: $Y_L = Y(W_i)$ and $Y_R = Y(W_{i+1})$. The matrix:

$$B(Y) = (W_{,Y}(Y))^{-1} A(W(Y)) W_{,Y}(Y)$$

($A(W)$ has the same eigenvalues as the Jacobian matrix of flux $F(W)$). Once the exact solution $Y^*(\frac{x}{t}; Y_L, Y_R)$ of this approximate problem (4.33) is obtained, the numerical flux is defined as:

$$\phi(W_L, W_R) = F(W(Y^*(0; Y_L, Y_R)))$$

Let us set \tilde{l}_k , $\tilde{\lambda}_k$ and \tilde{r}_k , $k = 1, \dots, p$, left eigenvectors, eigenvalues and right eigenvectors of matrix $B(\hat{Y})$ respectively. The solution $Y^*(\frac{x}{t}; Y_L, Y_R)$ of the linear Riemann problem is defined everywhere (except along $\frac{x}{t} = \tilde{\lambda}_k$):

$$\begin{aligned} Y^*\left(\frac{x}{t}; Y_L, Y_R\right) &= Y_L + \sum_{\frac{x}{t} > \tilde{\lambda}_k} ({}^t\tilde{l}_k \cdot (Y_R - Y_L)) \tilde{r}_k \\ &= Y_R - \sum_{\frac{x}{t} < \tilde{\lambda}_k} ({}^t\tilde{l}_k \cdot (Y_R - Y_L)) \tilde{r}_k \end{aligned}$$

or in a slightly different form:

$$Y_R - Y_L = \sum_{k=1,p} ({}^t\tilde{l}_k \cdot (Y_R - Y_L)) \tilde{r}_k = \sum_{k=1,p} \tilde{\alpha}_k \tilde{r}_k \quad (4.34)$$

setting:

$$\tilde{\alpha}_k = {}^t \tilde{l}_k \cdot (Y_R - Y_L)$$

The only remaining unknown is the mean \hat{Y} which must comply with the condition:

$$\hat{Y}(Y_l = Y_0, Y_r = Y_0) = Y_0$$

The standard average which is used is:

$$\hat{Y}(Y_L, Y_R) = (Y_L + Y_R)/2$$

The explicit form of the approximate Godunov scheme will be:

$$W_i^{n+1} - W_i^n + \frac{\Delta t}{\Delta x} (F(W(Y^*(0; Y_i^n, Y_{i+1}^n))) - F(W(Y^*(0; Y_{i-1}^n, Y_i^n)))) = 0$$

Remark 15 *A different prediction is obtained using instead:*

$$\hat{Y}(Y_L, Y_R) = Y^*(0; Y_L, Y_R)$$

where the approximate value at the interface $Y^*(0; Y_L, Y_R)$ is obtained solving (4.33) with:

$$\hat{Y}(Y_L, Y_R) = (Y_L + Y_R)/2$$

This correspond to the WFRoe-ncv scheme [29].

4.7.2 The classical VFRoe-ncv scheme for the interface model

We present here the VFRoe-ncv scheme for the system (4.24) using the variable $Z^\top = (C, \rho, U, P, Y)$. We denote by W the conservative variable, $W^\top = (\rho C, \rho, \rho U, \rho E, \rho Y)$. The Jacobian matrix associated to the flux $F(Z)^\top = (\rho U C, \rho U, \rho U^2 + P, U(\rho e(P, \rho, C, Y) + \rho U^2/2 + P), \rho U Y)$ is:

$$J(Z) = \begin{pmatrix} U & 0 & 0 & 0 & 0 \\ 0 & U & \rho & 0 & 0 \\ 0 & 0 & U & 1/\rho & 0 \\ 0 & 0 & \rho a^2 & U & 0 \\ 0 & 0 & 0 & 0 & U \end{pmatrix}$$

where a is defined by the formula (4.25).

Remark 16 *Note that because of the block-diagonal structure of $J(Z)$, it is easy to pick out information about the structure of the Jacobian of the HRM system (4.1) with a^2 define by (4.8) or the HEM system (4.14) with a^2 define by (4.19).*

The eigenvalues λ_i and the corresponding right eigenvectors r_i are:

$$\begin{aligned} \lambda_1 &= U - a; & r_1^\top &= (0, 1, -a/\rho, a^2, 0) \\ \lambda_2 &= U; & r_2^\top &= (1, 0, 0, 0, 0) \\ \lambda_3 &= U; & r_3^\top &= (0, 1, 0, 0, 0) \\ \lambda_4 &= U; & r_4^\top &= (0, 0, 0, 0, 1) \\ \lambda_5 &= U + a; & r_5^\top &= (0, 1, +a/\rho, a^2, 0) \end{aligned}$$

The matrix of the right eigenvector is $\Omega = (r_2, r_3, r_1, r_5, r_4)$ and:

$$\Omega(Z) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & -a/\rho & a/\rho & 0 \\ 0 & 0 & a^2 & a^2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\Omega(Z)^{-1} = \frac{-\rho}{2a^3} \begin{pmatrix} -2a^3/\rho & 0 & 0 & 0 & 0 \\ 0 & -2a^3/\rho & 0 & 2a/\rho & 0 \\ 0 & 0 & a^2 & -a/\rho & 0 \\ 0 & 0 & -a^2 & -a/\rho & 0 \\ 0 & 0 & 0 & 0 & -2a^3/\rho \end{pmatrix}$$

We defined the vector $\alpha^\top = (\alpha_2, \alpha_3, \alpha_1, \alpha_5, \alpha_4)$ as:

$$\alpha = \Omega(\bar{Z})^{-1}(Z_R - Z_L)$$

where Z_R and Z_L are the right and left states of the Riemann problem, and $\bar{Z} = \frac{Z_R + Z_L}{2}$ (other choices are possible). The solution of the linearized Riemann problem associated to $J(\bar{Z})$ and the states (Z_R, Z_L) is (see figure (4.10)),

$$Z(x/t; Z_L, Z_R) = Z_L + \sum_{\bar{\lambda}_i < x/t} \alpha_i \bar{r}_i = Z_R - \sum_{\bar{\lambda}_i > x/t} \alpha_i \bar{r}_i \quad (4.35)$$

with:

$$\bar{\lambda}_i = \lambda_i(\bar{Z}) \quad \text{and} \quad \bar{r}_i = r_i(\bar{Z})$$

This can be written in a slightly different form:

$$Z(x/t; Z_L, Z_R) = \begin{cases} Z_L & \text{if } x/t < \bar{\lambda}_1 \\ Z_1 & \text{if } \bar{\lambda}_1 < x/t < \bar{\lambda}_2 \\ Z_2 & \text{if } \bar{\lambda}_2 < x/t < \bar{\lambda}_5 \\ Z_R & \text{if } \bar{\lambda}_5 < x/t \end{cases}$$

We set $\Delta\Phi = \Phi_R - \Phi_L$. If we apply the formula (4.35) we find that the two intermediate states are:

$$Z_1 = \begin{pmatrix} C_L \\ \rho_L + \frac{\Delta P}{2\bar{a}^2} - \frac{\bar{\rho}\Delta U}{2\bar{a}} \\ \bar{U} - \frac{\Delta P}{2\bar{\rho}\bar{a}} \\ \bar{P} - \bar{\rho}\bar{a}\frac{\Delta U}{2} \\ Y_L \end{pmatrix} \quad Z_2 = \begin{pmatrix} C_R \\ \rho_R - \frac{\Delta P}{2\bar{a}^2} - \frac{\bar{\rho}\Delta U}{2\bar{a}} \\ \bar{U} - \frac{\Delta P}{2\bar{\rho}\bar{a}} \\ \bar{P} - \bar{\rho}\bar{a}\frac{\Delta U}{2} \\ Y_R \end{pmatrix}$$

In the above formulas \bar{a} is the sound speed calculated at the average state \bar{Z} , that is $\bar{a} = a(\bar{Z})$. The numerical flux for the classical VFRoe-ncv scheme is computed using $Z^* = Z(x/t = 0; Z_L, Z_R)$ (for example in the configuration of the figure (4.10) $Z^* = Z_1$).

Remark 17 – *The classical VFRoe-ncv scheme using variables (ρ, U, P) for the HEM model (4.14):*

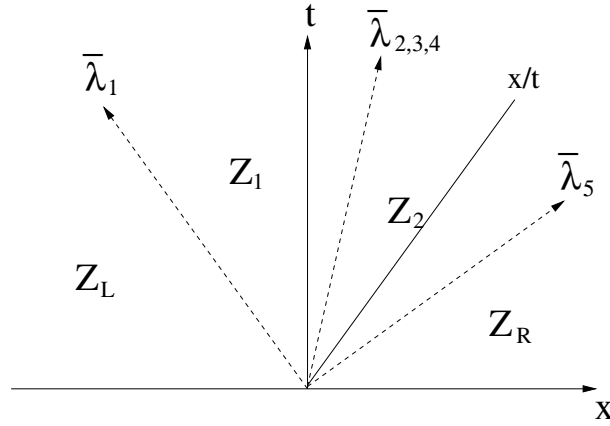


FIG. 4.10 – The four different states of the solution of the linearized Riemann problem

The linear Riemann Problem associated to the system (4.14) has two intermediate states as shown in figure (4.10). The intermediate states are:

$$Z_1 = \begin{pmatrix} \rho_L + \frac{\Delta P}{2\bar{a}_{HEM}^2} - \frac{\bar{\rho}\Delta U}{2\bar{a}_{HEM}} \\ \bar{U} - \frac{\Delta P}{2\bar{\rho}\bar{a}_{HEM}} \\ \bar{P} - \bar{\rho}\bar{a}_{HEM}\frac{\Delta U}{2} \end{pmatrix} \quad Z_2 = \begin{pmatrix} \rho_R - \frac{\Delta P}{2\bar{a}_{HEM}^2} - \frac{\bar{\rho}\Delta U}{2\bar{a}_{HEM}} \\ \bar{U} - \frac{\Delta P}{2\bar{\rho}\bar{a}_{HEM}} \\ \bar{P} - \bar{\rho}\bar{a}_{HEM}\frac{\Delta U}{2} \end{pmatrix}$$

– The classical VFRoe-ncv scheme using variables (C, ρ, U, P) for the HRM model (4.1): The linear Riemann Problem associated to the system (4.1) has two intermediate states as shown in figure (4.10). The intermediate states are:

$$Z_1 = \begin{pmatrix} C_L \\ \rho_L + \frac{\Delta P}{2\bar{a}_{HRM}^2} - \frac{\bar{\rho}\Delta U}{2\bar{a}_{HRM}} \\ \bar{U} - \frac{\Delta P}{2\bar{\rho}\bar{a}_{HRM}} \\ \bar{P} - \bar{\rho}\bar{a}_{HRM}\frac{\Delta U}{2} \end{pmatrix} \quad Z_2 = \begin{pmatrix} C_R \\ \rho_R - \frac{\Delta P}{2\bar{a}_{HRM}^2} - \frac{\bar{\rho}\Delta U}{2\bar{a}_{HRM}} \\ \bar{U} - \frac{\Delta P}{2\bar{\rho}\bar{a}_{HRM}} \\ \bar{P} - \bar{\rho}\bar{a}_{HRM}\frac{\Delta U}{2} \end{pmatrix}$$

4.7.3 The modified VFRoe-ncv scheme for the interface model

This modified VFRoe-ncv scheme for the interfacial model only differs from the classical VFRoe-ncv scheme in the choice of the average state which is not a classical average. We use here the "average state":

$$\tilde{Z}^\top = (\bar{C}, \bar{\rho}, \bar{U}, \bar{P}, \tilde{Y}); \quad \tilde{Y} = \begin{cases} 0 & \text{if } \bar{U} > 0 \\ 1 & \text{if } \bar{U} < 0 \end{cases}$$

This implies that the sound speed $\bar{a} = a(\bar{P}, \bar{\rho}, \bar{C}, \bar{Y})$ is replaced by,

$$\tilde{a} = \begin{cases} a_{HEM}(\bar{P}, \bar{\rho}) & \text{if } \bar{U} > 0 \\ a_{HRM}(\bar{P}, \bar{\rho}, \bar{C}) & \text{if } \bar{U} < 0 \end{cases}$$

This provides a new solution $Z^\#$ (note that $Y^\# = \tilde{Y}$). If we then explicit the numerical flux we find:

$$F(Z^\#)^\top = ((\rho UC)^\#, (\rho U)^\#, (\rho U^2 + P)^\#, (U(\rho e(P, \rho, C, Y) + \rho U^2/2 + P))^\#, (\rho UY)^\#)$$

with,

$$e^\# = \begin{cases} e_{HEM}(P^\#, \rho^\#) & \text{if } \bar{U} > 0 \\ e_{HRM}(P^\#, \rho^\#, C^\#) & \text{if } \bar{U} < 0 \end{cases}$$

Finally, if $\bar{U} > 0$ it is equivalent to apply the VFRoe-ncv scheme to the HEM system (4.23) with in addition the equations on Y and C of (4.24); and if $\bar{U} < 0$ it is equivalent to apply the VFRoe-ncv scheme to the HRM system (4.1) with in addition the equation on Y of (4.24).

Remark 18 *In the above modification of the classical VFRoe-ncv scheme we make a WFRoe-ncv scheme only for the domain variable Y .*

4.8 Appendix 2: Computation of C^{n+1} and P^{n+1} for the finite time relaxation step

In order to compute the finite relaxation step we need to explain how C^{n+1} and P^{n+1} are updated. They are the solution at the time Δt of the system (ODE) composed by the first and fourth equations of (4.30) with the initial condition: $C(t=0) = C^{\hat{n}}$ and $P(t=0) = P^{\hat{n}}$.

The main time step Δt is cut into N small uniform time steps $\delta t = \Delta t/N$. In the following C_i and P_i will stand for the successive approximations of C and P at the successive times $t = i \times \delta t$. Thus we will have:

$$\begin{aligned} C_0 &:= C^{\hat{n}} \text{ and } P_0 := P^{\hat{n}} \\ C^{n+1} &:= C_N \text{ and } P^{n+1} := P_N \end{aligned}$$

The chain rule which provides (C_{i+1}, P_{i+1}) in terms of (C_i, P_i) is the following:

- C_{i+1} is the *exact solution* at the time $t = \delta t$ of the ODE system:

$$\begin{cases} \frac{d}{dt}C(t) = \Gamma(P_i, \rho^{\hat{n}}, C(t)) \\ C(t=0) = C_i \end{cases} \quad (4.36)$$

where we have,

$$\Gamma(P_i, \rho^{\hat{n}}, C(t)) = (1 - C(t)) \left(C_{eq}(P_i, \rho^{\hat{n}}) - C(t) \right) \frac{1}{\Theta(P_i, \rho^{\hat{n}}, \tau_0)}$$

with the time scale,

$$\Theta(P, \rho, \tau_0) = \frac{\tau_0}{G_2(P, \rho)} \quad (4.37)$$

where G_2 defined by equation (4.10). We impose that the numerical approximation C_{i+1} respects the relations:

$$(C_{i+1} - C_{eq}(P_i, \rho^{\hat{n}}))(C_i - C_{eq}(P_i, \rho^{\hat{n}})) > 0 \quad (4.38)$$

$$(1 - C_{i+1})(1 - C_i) > 0 \quad (4.39)$$

This relation corresponds to the fact that the analytical solution $C(t)$ of (4.36) can not cross the poles $C = C_{eq}(P_i, \rho^{\hat{n}})$ and $C = 1$.

We get $C_{i+1} = C_i$ if $C_i = 1$ and if $C_i \neq 1$,

$$C_{i+1} = \frac{b_{i+1} + C_{eq}(P_i, \rho^{\hat{n}})}{1 + b_{i+1}} \quad (4.40)$$

with,

$$b_{i+1} = \frac{C_i - C_{eq}(P_i, \rho^{\hat{n}})}{1 - C_i} e^{(a_{i+1} \delta t)} \quad (4.41)$$

$$a_{i+1} = -(1 - C_{eq}(P_i, \rho^{\hat{n}})) \frac{G_2(P_i, \rho^{\hat{n}})}{\tau_0} \quad (4.42)$$

- To compute P_{i+1} , we use the fourth equation of the system (4.30) in the form

$$\partial_t (P) = -(\partial_P (e_{HRM}))^{-1} \partial_C (e_{HRM}) \partial_t (C)$$

and we make a rough integration:

$$P_{i+1} = P_i + \delta t (\partial_t (P))(P_i, \rho^{\hat{n}}, C_{i+1}, Y^{\hat{n}})$$

that is:

$$P_{i+1} = P_i - (C_{i+1} - C_i) \left(\frac{\partial_C (e_{HRM})}{\partial_P (e_{HRM})} \right) (P_i, \rho^{\hat{n}}, C_{i+1}, Y^{\hat{n}})$$

A numerical maximum principle :

We assume that $C_{eq}(P_i, \rho^{\hat{n}})$ remains in $[0,1]$.

- We assume that $0 \leq C_{eq}(P_i, \rho^{\hat{n}}) \leq C_i \leq 1$:

This implies that $b_{i+1} \geq 0$. Hence using the equation (4.40) we get:

$$0 \leq C_{i+1} \leq 1$$

- We assume that $0 \leq C_i \leq C_{eq}(P_i, \rho^{\hat{n}}) \leq 1$:

This implies that $b_{i+1} \leq 0$. We set,

$$H(b) = \frac{b + C_{eq}(P_i, \rho^{\hat{n}})}{1 + b} \quad \text{and} \quad J(b) = 1 - H(b)$$

We thus have $H(b_{i+1}) = C_{i+1}$ and $J(b_{i+1}) = 1 - C_{i+1}$. When we examine the positivity of both $H(b)$ and $J(b)$ we find that it is equivalent to the relation $b \geq -C_{eq}(P_i, \rho^{\hat{n}})$. This latter leads to the condition on the time step δt :

$$\delta t \geq 0$$

which is obviously respected.

Hence we get for $\delta t \geq 0$:

$$0 \leq C_{i+1} \leq 1$$

We thus have the following property.

Property:

The following maximum principle holds for the finite time relaxation step. If we assume that:

- (i) the time step δt is positive,
- (ii) the pole $C_{eq}(P_i, \rho^{\hat{n}})$ of the ODE system (4.36) remains in $[0,1]$,
- (iii) $0 \leq C_i \leq 1$

Then we have $0 \leq C_{i+1} \leq 1$.

Remark 19 *Actually, the only assumption is that $C_{eq}(P_i, \rho^{\hat{n}})$ remains in $[0,1]$. The finite time relaxation step does not ensure that $C_{eq}(P_{i+1}, \rho^{\hat{n}})$ will remain in $[0,1]$ (see appendix 4 for similar comments on C_{eq}).*

4.9 Appendix 3: On the discrete preservation of contact waves in HEM and HRM models

4.9.1 HRM

This paragraph is strongly connected with the section dealing with the numerical schemes. It refers to the work exposed in [30]. We formally set $\Gamma = 0$ in the system (4.1). A pure contact solution is an analytical solution of (4.1) (with $\Gamma = 0$) of the form:

$$\begin{cases} C(x,t) = C_0(x - U_0t) \\ \rho(x,t) = \rho_0(x - U_0t) \\ U(x,t) = U_0 \\ P(x,t) = P_0 \end{cases} \quad (4.43)$$

When the initial condition is such that the pressure and the velocity are uniform, the initial profiles of C and density (i.e. $C_0(x)$ and $\rho_0(x)$) are advected with speed U_0 . We say that the contact solution is preserved by the conservative numerical scheme if the numerical approximation of the velocity and the pressure remain constant in each cell of the discrete domain.

According to [30], the discrete contact solution is respected if two conditions are fulfilled:

(i) The internal energy must be of the form:

$$\rho e = f_1(P) + \rho f_2(P) + \rho C f_3(P) \quad (4.44)$$

(ii) The numerical flux involved in the conservative scheme preserves the contact solution.

Remark 20 *The second point (ii) is achieved when using either the Godunov scheme or VFRoe-ncv scheme with variables (C, ρ, U, P) .*

The two conditions are necessary to preserve the discrete profiles of both U and P . If (i) is not fulfilled, the contact solution will not be respected whatever the conservative numerical scheme is (even for the Godunov scheme). We insist that whatever the continuous function defining the EOS (i.e. $(P, \rho, C) \mapsto e_{HRM}(P, \rho, C)$) for the HRM model is, the vector (4.43) is an analytical solution of the system (4.1) without any source term.

Rewriting (4.5) we find that the internal energy is of the form:

$$\rho e = \phi_1(P) + \rho \phi_2(P) + \rho C (-\phi_2(P)) \quad (4.45)$$

with:

$$\begin{aligned} \phi_1(P) &= (\delta_l - 1)P \\ \phi_2(P) &= \left[\left(1 - \frac{\delta_l}{\delta_v}\right) h_v^s(P) \right] \end{aligned}$$

Hence this internal energy allows the discrete preservation of the contact wave since the condition (i) is fulfilled. In our numerical tests the convective part of the HRM model will be computed using a VFRoe-ncv scheme with variables (C, ρ, U, P) that fulfills the condition (ii) (see [30]).

4.9.2 HEM

The internal energy of the HEM model takes the form:

$$\rho e = \phi_4(P) + \rho\phi_5(P) \quad (4.46)$$

with:

- In the pure liquid domain D_l :

$$\phi_4(P) = (\delta_l - 1)P \quad \text{and} \quad \phi_5(P) = 0$$

- In the two-phase domain $D_{2\Phi}$:

$$\phi_4(P) = \left[-P + \frac{h_v^s(P) - h_l^s(P)}{\tau_v^s(P) - \tau_l^s(P)} \right]$$

$$\phi_5(P) = \left[\frac{\tau_v^s(P)h_l^s(P) - \tau_l^s(P)h_v^s(P)}{\tau_v^s(P) - \tau_l^s(P)} \right]$$

Following [30], we conclude that this EOS allows the preservation of the discrete contact solution in the pure HEM domain. Hence when the discrete contact solution evolves in a single domain (i.e. in the pure liquid or in the two-phase domain), it is preserved provided that the numerical scheme preserves the contact solution. This is not true anymore when going through the boundary between the domains $D_{2\Phi}$ and D_l (a numerical example is available in [55]).

4.9.3 Contact waves travelling through the coupling interface

We know that the discrete contact solutions are preserved by the HEM and the HRM models. We examine herein what happens when a contact wave hits the coupling interface (as described by figure (4.11)).

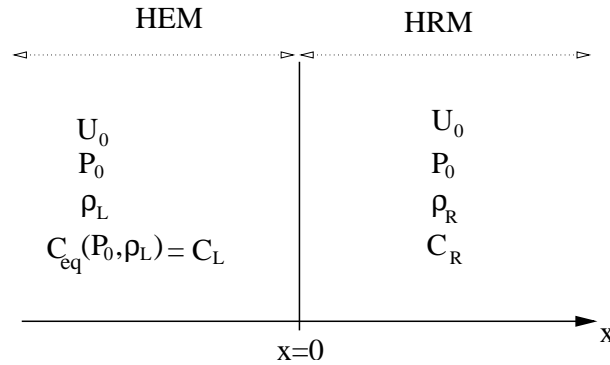


FIG. 4.11 – Initial data for a contact test case hitting the coupling interface

Remark 21 Thanks to the preservation of the contact wave for sole HEM and HRM models, we only need to examine the discrete values of the variables in the two cells on each side of the coupling interface.

- a) $U_0 > 0$

A problem may only occurs in the first cell in the HRM domain. After one time step of our coupling scheme involving VFRoe-ncv scheme and described above in appendix 1, we get in the first cell of the HRM domain the values (ρ, U, P, C) defined by:

$$\rho - \rho_R + \lambda(\rho_R U_0 - \rho_L U_0) = 0 \quad (4.47)$$

$$\rho U - \rho_R U_0 + \lambda(\rho_R U_0^2 + P_0 - \rho_L U_0^2 - P_0) = 0 \quad (4.48)$$

$$\rho E_{HRM} - \rho_R E_{HRM}^R + \lambda(U_0(\rho_R E_{HRM}^R + P_0) - U_0(\rho_L E_{HEM}^L + P_0)) = 0 \quad (4.49)$$

$$\rho C - \rho_R C_R + \lambda(\rho_R U_0 C_R - \rho_L U_0 C_{eq}^L) = 0 \quad (4.50)$$

with $\lambda = \frac{\Delta t}{\Delta x}$ and:

$$E_{HRM} = e_{HRM}(P, \rho, C) + \frac{U^2}{2}$$

$$E_{HRM}^R = e_{HRM}(P_0, \rho_R, C_R) + \frac{U_0^2}{2}$$

$$E_{HEM}^L = e_{HEM}(P_0, \rho_L) + \frac{U_0^2}{2} = e_{HRM}(P_0, \rho_L, C_{eq}^L) + \frac{U_0^2}{2}$$

$$C_{eq}^L = C_{eq}(P_0, \rho_L)$$

Using the internal energy in the form (4.45), the system (4.47)-(4.50) provides:

$$\rho - \rho_R + \lambda U_0(\rho_R - \rho_L) = 0 \quad (4.51)$$

$$U = U_0 \quad (4.52)$$

$$(\Phi_1(P) - \Phi_1(P_0)) + \rho(1 - C)(\Phi_2(P) - \Phi_2(P_0)) = 0 \quad (4.53)$$

$$\rho C - \rho_R C_R + \lambda(\rho_R U_0 C_R - \rho_L U_0 C_{eq}^L) = 0 \quad (4.54)$$

The equation (4.53) implies that for any $\rho \geq 0$ and for any $\rho(1 - C) \geq$ defined by (4.51) and (4.54):

$$\Phi_1(P) = \Phi_1(P_0) \quad \text{and} \quad \Phi_2(P) = \Phi_2(P_0)$$

and thanks to the bijectivity of the applications $P \mapsto \Phi_1(P)$ and $P \mapsto \Phi_2(P)$ this leads to $P = P_0$.

Thus the contact wave passing from the HEM model to the HRM model will be preserved.

b) $U_0 < 0$

A problem may only occur in the first cell in the HEM domain. One time step of the coupling described above provides in the first cell of the HEM domain the values (ρ, U, P) defined by:

$$\rho - \rho_L + \lambda(\rho_R U_0 - \rho_L U_0) = 0 \quad (4.55)$$

$$\rho U - \rho_L U_0 + \lambda(\rho_R U_0^2 + P_0 - \rho_L U_0^2 - P_0) = 0 \quad (4.56)$$

$$\rho E_{HEM} - \rho_L E_{HEM}^L + \lambda(U_0(\rho_R E_{HRM}^R + P_0) - U_0(\rho_L E_{HEM}^L + P_0)) = 0 \quad (4.57)$$

with $\lambda = \frac{\Delta t}{\Delta x}$ and:

$$E_{HEM} = e_{HEM}(P, \rho) + \frac{U^2}{2}$$

$$E_{HRM}^R = e_{HRM}(P_0, \rho_R, C_R) + \frac{U_0^2}{2}$$

$$E_{HEM}^L = e_{HEM}(P_0, \rho_L) + \frac{U_0^2}{2}$$

Using the internal energy in the form (4.46), the system (4.55)-(4.57) provides:

$$\rho - \rho_L + \lambda(\rho_R U_0 - \rho_L U_0) = 0 \quad (4.58)$$

$$U = U_0 \quad (4.59)$$

$$\Phi_4(P) - \Phi_4(P_0) + \rho(\Phi_5(P) - \Phi_5(P_0)) + \lambda U_0 \rho_R (e_{HRM}^R - e_{HEM}^R) = 0 \quad (4.60)$$

Hence if $P = P_0$, the equation (4.60) reads:

$$e_{HRM}(P_0, \rho_R, C_R) = e_{HRM}(P_0, \rho_R, C_{eq}^R)$$

which thanks to the bijectivity of $C \mapsto e_{HRM}(P, \rho, C)$ implies that $C_R = C_{eq}^R$. Then a necessary condition for the respect of the discrete contact solution is:

$$C_R = C_{eq}(P_0, \rho_R)$$

Let us now assume that $C_R = C_{eq}(P_0, \rho_R)$. Thus $e_{HRM}(P_0, \rho_R, C_R) = e_{HRM}(P_0, \rho_R, C_{eq}^R)$, and the pressure P is a solution of the equation:

$$\Phi_4(P) - \Phi_4(P_0) + \rho(\Phi_5(P) - \Phi_5(P_0)) = 0 \quad (4.61)$$

where ρ is defined by the equation (4.58). The preceding equation must be fulfilled for any ρ . Thus it implies that

$$\Phi_4(P) = \Phi_4(P_0) \quad \text{and} \quad \Phi_5(P) = \Phi_5(P_0) \quad (4.62)$$

The two equations of (4.62) can be rewritten as second order polynomials with respect to the variable P . Obviously P_0 is one solution. It can be shown that the second solution of the second equation of (4.62) is greater than P_{MAX} for all P_0 in $[P_{MIN}, P_{MAX}]$. Thus the second equation of (4.62) has a unique admissible solution $P = P_0$. This implies that $P = P_0$ is the unique solution of the system (4.62). We can deduce that $C_R = C_{eq}(P_0, \rho_R)$ is a sufficient condition for the preservation of the contact wave.

Finally, the condition $C_R = C_{eq}(P_0, \rho_R)$ is a necessary and sufficient condition to fulfill for the preservation of the discrete contact wave when hitting the coupling interface.

4.10 Appendix 4: Positivity results for the HRM model

Let us begin by recalling a classical lemma.

Lemma:

Let Ω be a subset of R^n . Let Ψ , a , Π and U be some sufficiently regular applications, with properties:

- $\Psi : (\Omega \times [0, T] \rightarrow R, (x, t) \rightarrow \Psi(x, t))$.
- $a : (\Omega \times [0, T] \rightarrow R, (x, t) \rightarrow a(x, t)), a \in L^\infty$.
- $\Pi : (\Omega \times [0, T] \rightarrow R, (x, t) \rightarrow \Pi(x, t)), \Pi \geq 0$.
- $U : (\Omega \times [0, T] \rightarrow R^n, (x, t) \rightarrow U(x, t)), U \in L^\infty$ and $Div(U) \in L^\infty$.

and such that:

$$\partial_t (\Psi(x, t)) + U \partial_x (\Psi(x, t)) = a(x, t) \Psi(x, t) + \Pi(x, t) \quad (4.63)$$

Suppose that on $\partial\Omega$, the boundary of Ω , $\Psi^-(x, t) = 0$ if $(U \cdot n)(x, t) \leq 0$, where n is the outward normal of Ω . With all this assumptions, if $\Psi(x, t = 0) \geq 0$ then for all $0 \leq t \leq T$, $\Psi(x, t) \geq 0$.

In the following we will assume that:

$$U \in L^\infty \quad \text{and} \quad Div(U) \in L^\infty$$

a) Evolution of the density ρ :

The lemma applies to the second equation of (4.11). It ensures the positivity of the total density ρ :

$$\rho \geq 0$$

b) Evolution of the pressure P :

b.1) The fourth equation of (4.11) can take the form:

$$\partial_t (P) + U \partial_x (P) + \hat{\gamma} P \partial_x (U) = PJ(P, \rho, C)$$

where the term $J(P, \rho, C)$ is bounded if ρ is bounded and if $\rho(1 - C)$ remains positive. The lemma thus applies and we get:

$$P > 0 \text{ if } \rho \text{ is bounded and } \rho(1 - C) > 0$$

b.2) The fourth equation of (4.11) does not ensure that P remains in $[P_{MIN}, P_{MAX}]$. This equation can be written:

$$\partial_t (P) + U \partial_x (P) + \hat{\gamma} P \partial_x (U) = (1 - C)(\bar{C} - C)F(P, \rho)$$

where F is positive for $P \in [P_{MIN}, P_{MAX}]$ and $\rho > 0$. Hence if we choose $P(x, t = 0) = P_{MIN}$, $U(x, t = 0) = U_0$, $\rho(x, t = 0) = \rho_0$ and $C(x, t = 0) = C_0$ with the relation $C_0 < \bar{C}(P_0, \rho_0) < 1$, then:

$$\partial_t (P)|_{t=0} < 0$$

Thus $P(x, t = 0^+) < P_{MIN}$. We may also choose initial conditions such that $P(x, t = 0^+) > P_{MAX}$. In fact, this makes sense since the only physically relevant lower and upper bounds for the pressure are $P_{MIN} = 0$, and $P_{MAX} = P_{critical}$. As discussed above, this particular value of the lower bound

will not lead to any problem. The problem is actually less obvious with the upper bound since our governing equations probably no longer make sense around the critical point.

c) Evolution of the liquid mass fraction C :

We make the assumption that ρ is bounded and that $P \in [P_{MIN}, P_{MAX}]$. It implies that G_2 is bounded.

We set $\Psi_1 = 1 - C$. Then the first equation of the system (4.11), gives:

$$\partial_t (\Psi_1) + U \partial_x (\Psi_1) = -\Psi_1(x,t)(\bar{C} - C) \frac{G_2(P,\rho)}{\tau_0}$$

By applying the lemma mentioned above we find that $C < 1$.

We set now $\Psi_2 = C$. Then the first equation of the system (4.11), gives:

$$\partial_t (\Psi_2) + U \partial_x (\Psi_2) = \Psi_2(x,t)(C - 1) \frac{G_2(P,\rho)}{\tau_0} + \Pi$$

with $\Pi = \bar{C}(1 - C) \frac{G_2(P,\rho)}{\tau_0}$. If we make the assumption that $\bar{C} > 0$, the source term Π is always positive. By applying the lemma we find that $C > 0$.

$C < 1$ if ρ is bounded and $P \in [P_{MIN}, P_{MAX}]$ $C > 0$ if ρ is bounded, $P \in [P_{MIN}, P_{MAX}]$ and $\bar{C} > 0$

d) Evolution of the liquid mass fraction \bar{C} :

Owing to the latter result, we wonder whether \bar{C} remain in $[0,1]$. We have the equivalence:

$$0 < \bar{C} < 1 \iff \tau_l^s(P) < \tau < \tau_v^s(P)$$

We set $\Psi_3 = \tau_v^s(P) - \tau$ and $\Psi_4 = \tau - \tau_l^s(P)$. The governing equations for Ψ_3 and Ψ_4 are:

$$\partial_t (\Psi_3) + U \partial_x (\Psi_3) - \Psi_3 \partial_x (U) + (\hat{\gamma} P \frac{d}{dP} \tau_v^s(P) + \tau_v^s(P)) \partial_x (U) = -\frac{\partial_C (e_{HRM})}{\partial_P (e_{HRM})} \Gamma \frac{d}{dP} \tau_v^s(P) \quad (4.64)$$

$$\partial_t (\Psi_4) + U \partial_x (\Psi_4) - \Psi_4 \partial_x (U) - (\hat{\gamma} P \frac{d}{dP} \tau_l^s(P) + \tau_l^s(P)) \partial_x (U) = \frac{\partial_C (e_{HRM})}{\partial_P (e_{HRM})} \Gamma \frac{d}{dP} \tau_l^s(P) \quad (4.65)$$

Hence the lemma cannot be applied. Moreover we can choose initial data such that $\bar{C} > 1$ or $\bar{C} < 0$. For example with $P(x,t=0) = P_0$, $U(x,t=0) = U_0$, $\rho(x,t=0) = 1/\tau_v^s(P_0)$ and $C(x,t=0) = C_0$ with $C_0 \in]\bar{C}(P_0, \rho_0), 1[$ the equation (4.64) gives:

$$\partial_t (\Psi_3)|_{t=0} < 0$$

with $\Psi_3|_{t=0} = 0$. Then $\Psi_3|_{t=0+} < 0$ and $\bar{C}|_{t=0+} < 0$. We may also choose initial conditions such that $\bar{C}|_{t=0+} > 1$.

Let us assume that there are no source terms, $\Gamma = 0$. A sufficient condition for \bar{C} to remain in $[0,1]$ is to have:

$$\begin{cases} \hat{\gamma} P \frac{d}{dP} \tau_v^s(P) + \tau_v^s(P) = 0 \\ \hat{\gamma} P \frac{d}{dP} \tau_l^s(P) + \tau_l^s(P) = 0 \end{cases} \quad (4.66)$$

which implies, thanks to our closure laws:

$$A_v B_l - A_l B_v = 0 \quad (4.67)$$

Moreover, if we assume that $\frac{d}{dP} h_v^s \leq 0$ and $\frac{d}{dP} h_v^s \geq 0$, the sole possibility is to have horizontal lines in the (P, h) plane:

$$h_l^s = B_l \quad \text{and} \quad h_v^s = B_v \quad (4.68)$$

Moreover, (4.66) together with (4.68) implies: $\gamma_L = 1$.

We refer to the work of Jaouen [57] and also to the work of Caro [17] for similar discussions on problems that are connected with thermodynamics for two-phase flow.

e) Evolution of the liquid density ρ_l :

If we assume that $C > 0$, then:

$$\rho_l \geq 0 \iff \tau \geq \tau_v^s(P)(1 - C)$$

We set $\Psi_5 = \tau - \tau_v^s(P)(1 - C)$. The density ρ_l and the function Ψ_5 have then the same sign. The governing equation on Ψ is:

$$\partial_t (\Psi_5) + U \partial_x (\Psi_5) - \left[(1 - C) \hat{\gamma} P \frac{d}{dP} \tau_v^s(P) + \tau \right] \partial_x (U) = (1 - C) \frac{\partial_C (e_{HRM})}{\partial_P (e_{HRM})} \Gamma \frac{d}{dP} \tau_v^s(P) + \Gamma \tau_v^s(P)$$

As in subsection *d*) or *b*), this equation allows Ψ_5 to be positive or negative. Thus nothing ensures that ρ_l remains positive.

Chapitre 5

Couplage interfacial d'un modèle homogène et d'un modèle bi-fluide

Dans le domaine de la production nucléaire civile, deux approches sont possibles aujourd'hui pour assurer la simulation industrielle des écoulements diphasiques possédant une phase vapeur et une phase liquide. Le premier type de modèle rassemble les modèles homogénéisés. Ceux-ci ont la particularité de représenter les deux fluides sous la forme d'un fluide unique dont les propriétés seraient des moyennes des propriétés des deux phases isolées. Les équations aux dérivées partielles portent alors sur des grandeurs de mélange. C'est dans cette classe de modèles que se rangent les modèles HEM et HRM utilisés au chapitre 4. La seconde approche regroupe les modèles bi-fluides. Ils ont la particularité de considérer les deux fluides séparément. Chaque phase possède ses propres grandeurs physiques associées à un jeu d'équations qui lui est propre. Le "couplage" des deux phases est assuré par des grandeurs interfaciales (pression et vitesse interfaciales) et des échanges interfaciaux (transferts de masse, effets de trainée, transferts d'énergie). Le modèle à une pression bi-fluide standard à six équations, ainsi que le modèle bi-fluide à deux pressions entrent dans cette catégorie.

Nous nous proposons dans ce chapitre d'appliquer une méthode de couplage, reprenant certains principes des méthodes développées aux chapitres 3 et 4, au cas du couplage interfacial instationnaire du modèle bi-fluide standard à six équations et d'un modèle HRM (comportant 4 équations). Le couplage ainsi que la dérivation des modèles à coupler sont assurés grâce au modèle bi-fluide à deux pressions. La dérivation et la simulation du modèle bi-fluide standard sont réalisées grâce à la méthode de relaxation décrite en annexe C. Une méthode similaire est appliquée pour calculer les approximations discrètes d'un modèle HRM à quatre équations à partir du modèle bi-fluide à deux pressions. Le couplage interfacial de ces deux modèles est assuré par le modèle "père" bifluide à deux pressions. Une particularité de cette démarche par rapport à la démarche du chapitre 4 est d'assurer implicitement la compatibilité thermodynamique entre les modèles. De ce fait la variable de domaine (ou couleur) Y n'intervient pas dans la définition de la loi d'état du modèle père; elle apparaît uniquement dans la définition des termes sources.

Une version industrielle de ce couplage a par ailleurs été réalisée en couplant un modèle HRM au code de calcul NEPTUNE_CFD basé sur le modèle bi-fluide standard (voir rapport [54]). Bien que les méthodes numériques soient différentes pour les deux codes (prédicteur/correcteur en pression pour NEPTUNE_CFD et schéma hyperbolique pour HRM), le comportement de l'algorithme de couplage est très encourageant.

Couplage interfacial d'un modèle homogène et d'un modèle bi-fluide

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Abstract : On propose dans ce chapitre une technique de couplage du code NEPTUNE_CFD, qui propose des approximations des solutions du modèle bifluide à un champ de pression, avec un code de simulation d'écoulement diphasique homogène. Le principe général repose sur l'utilisation du modèle diphasique hyperbolique à deux champs de pression.

5.1 Introduction

Dans le cadre du projet NEPTUNE, un des objectifs visés consiste à effectuer un couplage d'un code tel que CATHARE ou NEPTUNE_CFD (modèle bi-fluide à six équations) à un code composant (modèle homogène à quatre équations), le code composant étant censé donner une représentation de la partie coeur, tandis que le modèle le plus complexe assure la description du fluide caloporteur dans les conduites du circuit primaire. L'échelle de description n'est pas la même dans les deux cas: la taille représentative dans la conduite est de l'ordre du mètre, celle dans le coeur étant de l'ordre du sous-canal (approximativement 1 cm). Pour aborder ce problème très complexe de couplage interfacial, on choisit de procéder en deux temps. On définit tout d'abord une stratégie d'ensemble sur une configuration académique, où les deux codes et l'algorithme de couplage sont développés en totalité. Dans un second temps, il s'agira d'utiliser l'algorithme de couplage précédemment défini, pour l'appliquer au cas de couplage réel. Le code retenu pour la simulation du modèle bi-fluide sera le code NEPTUNE_CFD.

Contrairement au chapitre 4, la technique de base qui sera utilisée s'inspirera des idées développées dans l'article [44], et non pas du formalisme proposé dans [39]. On considérera un modèle père basé sur le modèle bi-fluide à sept équations. Il faut signaler que ce choix de cadre de modèles n'est pas classique dans la communauté diphasique actuelle.

Les modèles bi-fluides à deux pressions ont été introduits dans le cadre de la DDT, et leur application au cadre des écoulements de type eau-vapeur n'a été envisagée que plus récemment. On pourra notamment consulter les références [12], [60],[69] pour l'aspect gaz-particules, et par exemple [64], [35], [34], concernant la modélisation de ces écoulements dans le cadre eau-vapeur. Le principe sous-jacent dans ce chapitre est d'utiliser ce formalisme de représentation des écoulements diphasiques en l'associant aux techniques de relaxation ([14], [15], [7], [19]), pour effectuer la simulation des deux modèles à coupler, mais aussi pour définir l'algorithme de couplage de ces deux modèles.

On présente tout d'abord de manière succincte le modèle global (section 2), en introduisant les termes physiques de transfert de masse, de quantité de mouvement et d'énergie. Ceux-ci sont en outre indispensables à l'obtention des deux modèles à coupler. Les termes de relaxation en vitesse, pression et température qui apparaîtront vont permettre de "projeter" le modèle père sur le modèle homogène et sur le modèle bi-fluide à une pression. Ces formes de termes sources sont choisies pour être conformes à l'inégalité d'entropie, point qui est fondamental pour notre approche. Signalons que ces arguments ont également été retenus dans le cadre [46] et [50].

En ce qui concerne les fermetures associées aux vitesses et pressions interfaciales, l'argument principal retenu correspond à l'hypothèse de champ linéairement dégénéré associé à la valeur propre V_I , proposée dans [25], [34]. Une propriété essentielle qui en découle concerne la définition d'un unique jeu de relations de saut, ce qui est tout à fait remarquable dans le cadre des modèles bi-fluides (une conséquence immédiate étant que les solutions chocs convergées sont indépendantes des schémas utilisés, voir par exemple [46]).

La simulation du modèle bi-fluide et du modèle homogène (sections 5.3 et 5.4) se déduit alors simplement en relaxant instantanément en pression et en pression/vitesse/température respectivement. En outre, seule la partie convective du modèle père intervient dans l'algorithme de couplage (section 5.5). Le traitement numérique du système d'évolution et des étapes de relaxation physique et de relaxation instantanée est décrit en détail. Plusieurs simulations de cas tests unidimensionnels et bidimensionnels permettent d'évaluer les capacités de l'approche proposée (section 5.6).

5.2 Présentation du modèle bi-fluide à deux pressions

Le système d'équations du modèle bi-fluide à deux pressions est constitué de sept équations. Chacune des deux phases est décrite à l'aide d'une équation de conservation de la masse, d'une équation de conservation de la quantité de mouvement et d'une équation de conservation de l'énergie phasique totale; on adjoint à ces six équations une équation de transport de la fraction volumique d'une des phases. Les deux phases seront distinguées par les indices v pour la phase vapeur et l pour la phase liquide. Les échanges entre les deux phases sont pris en compte par les terme sources d'ordre zéro $S_{k,\phi}$ pour $k = 2,3,4$ et $\phi = l,v$. Le système bi-fluide à deux pressions s'écrit :

$$\left\{ \begin{array}{l} \partial_t (\alpha_l) + V_I \partial_x (\alpha_l) = S_{1,l} \\ \partial_t (\alpha_l \rho_l) + \partial_x (\alpha_l \rho_l U_l) = S_{2,l} \\ \partial_t (\alpha_l \rho_l U_l) + \partial_x (\alpha_l \rho_l U_l^2 + \alpha_l P_l) - P_I \partial_x (\alpha_l) = S_{3,l} \\ \partial_t (\alpha_l E_l) + \partial_x (\alpha_l U_l (E_l + P_l)) + P_I \partial_t (\alpha_l) = S_{4,l} \\ \partial_t (\alpha_v \rho_v) + \partial_x (\alpha_v \rho_v U_v) = S_{2,v} \\ \partial_t (\alpha_v \rho_v U_v) + \partial_x (\alpha_v \rho_v U_v^2 + \alpha_v P_v) - P_I \partial_x (\alpha_v) = S_{3,v} \\ \partial_t (\alpha_v E_v) + \partial_x (\alpha_v U_v (E_v + P_v)) + P_I \partial_t (\alpha_v) = S_{4,v} \end{array} \right. \quad (5.1)$$

où les variables sont :

- les fractions volumiques des phases liquide α_l et vapeur α_v , reliées par la relation $\alpha_l + \alpha_v = 1$;
- les densités des phases liquide ρ_l et vapeur ρ_v ;
- les vitesses des phases liquide U_l et vapeur U_v ;
- les pressions au sein des phases liquide P_l et vapeur P_v .

Par ailleurs les énergies totales phasiques E_l et E_v s'expriment en fonction des énergies internes e_v et e_l ainsi que des énergies cinétiques phasiques :

$$E_\phi = \rho_\phi e_\phi(P_\phi, \rho_\phi) + \rho_\phi \frac{U_\phi^2}{2}, \quad \phi = v, l \quad (5.2)$$

La loi thermodynamique de chacun des fluides est choisie dans la classe des gaz raides, c'est-à-dire que l'énergie interne s'écrit :

$$(\gamma_\phi - 1) \rho_\phi e_\phi = P_\phi + \gamma_\phi P_{\infty, \phi}, \quad \phi = v, l \quad (5.3)$$

A chaque phase $\phi = l, v$ est associée une entropie $s_\phi(P_\phi, \rho_\phi)$ définie par l'équation aux dérivées partielles suivante :

$$\hat{\gamma}_\phi P_\phi \partial_{P_\phi} (s_\phi) + \rho_\phi \partial_{\rho_\phi} (s_\phi) = 0 \quad (5.4)$$

où le terme $\hat{\gamma}_\phi P_\phi = (\partial_{P_\phi} (e_\phi)|_{\rho_\phi})^{-1} (P_\phi / \rho_\phi - \rho_\phi \partial_{\rho_\phi} (e_\phi)|_{P_\phi})$ permet de définir la célérité c_ϕ du son dans chacune des phases :

$$\hat{\gamma}_\phi P_\phi = \rho_\phi c_\phi^2$$

Remarque. Si une entropie s_ϕ vérifie l'équation (5.4), alors pour toute fonction G de $C^1(\mathbb{R})$ strictement monotone $G(s_\phi)$ vérifiera (5.4).

On considère l'entropie phasique :

$$s_\phi = C_{V,\phi} \ln \left(\frac{P_\phi + P_{\infty,\phi}}{\rho_\phi^{\gamma_\phi}} \right) \quad (5.5)$$

ainsi que la température phasique dont la définition générale est :

$$T_\phi^{-1} = \partial_{e_\phi} (s_\phi)|_{\rho_\phi}$$

Dans notre cas la température phasique s'écrit donc :

$$T_\phi = \frac{P_\phi + P_{\infty,\phi}}{\rho_\phi C_{V,\phi}(\gamma_\phi - 1)} \quad (5.6)$$

La partie convective du système (5.1) est inconditionnellement hyperbolique mais ne peut s'écrire sous forme conservative. Il reste à choisir les fermetures associées au couple (V_I, P_I) ainsi que les termes sources $S_{k,\phi}$ pour $k = 1,2,3,4$ et $\phi = l,v$.

La procédure qui a été considérée est la suivante (voir [25] , [34]):

1. En l'absence de terme source, l'interface entre les phases ne peut s'épaissir sous le seul effet des termes convectifs. Dès lors le champ associé à V_I est linéairement dégénéré (c'est-à-dire le champ associé à α_ϕ).
2. On présuppose, en retenant la forme classique des termes de diffusion (loi de Fourier pour l'équation d'énergie et la fermeture classique à un paramètre en loi de premier gradient pour la viscosité dynamique) une forme prédéfinie du bilan d'entropie physique pour le système à sept équations.

On obtient ainsi les fermetures suivantes :

1. de la première hypothèse on déduit la loi de vitesse interfaciale :

$$V_I = \delta U_l + (1 - \delta)U_v \quad (5.7)$$

avec trois choix possibles pour le paramètre δ ,

$$\delta = 0 \quad \text{ou} \quad \delta = 1 \quad \text{ou} \quad \delta = \frac{\alpha_l \rho_l}{\alpha_l \rho_l + \alpha_v \rho_v} \quad (5.8)$$

2. en ajoutant la seconde hypothèse on en déduit la loi liant la pression interfaciale P_I à la vitesse interfaciale V_I :

$$P_I = \frac{(1 - \delta)a_l P_l + \delta a_v P_v}{(1 - \delta)a_l + \delta a_v} \quad (5.9)$$

en notant,

$$a_\phi = (\partial_{P_\phi} (e_\phi)|_{\rho_\phi})^{-1} \partial_{P_\phi} (s_\phi)|_{\rho_\phi}, \quad \phi = l,v$$

ce qui donne dans notre cas :

$$a_\phi = T_\phi^{-1}, \quad \phi = l,v$$

Remarque essentielle. Une fois que le choix du δ est fait (5.8), la fermeture des relations de saut est unique.

Le bilan d'entropie est le suivant :

$$\partial_t (\eta) + \partial_x (F_\eta) < 0$$

où le couple entropie-flux d'entropie est défini grâce aux entropies phasiques,

$$\eta = -(\alpha_v \rho_v s_v + \alpha_l \rho_l s_l) \quad \text{et} \quad F_\eta = -(\alpha_v \rho_v s_v U_v + \alpha_l \rho_l s_l U_l)$$

Remarque. *Cette entropie est convexe mais pas strictement convexe. Pour obtenir une stricte convexité, il faudrait introduire une contribution d'entropie d'interface.*

Il reste uniquement à ce stade à donner la forme des termes sources $S_{k,\phi}$. Seuls seront considérés les termes de transfert interfacial. Dès lors les termes $S_{k,\phi}$ doivent satisfaire les contraintes

$$S_{k,l} + S_{k,v} = 0 \quad \text{pour} \quad k = 2,3,4$$

On détermine des formes admissibles de ceux-ci de sorte que l'inégalité d'entropie physique précédente reste inchangée.

$$\begin{aligned} S_{1,l} &= \mathcal{A} \\ S_{2,l} &= \Gamma \\ S_{3,l} &= \mathcal{B} + V_I \Gamma \\ S_{4,l} &= \mathcal{C} + V_I \mathcal{B} + H_I \Gamma \end{aligned} \tag{5.10}$$

où les termes \mathcal{A} , \mathcal{B} , \mathcal{C} et Γ sont définis comme suit :

$$\begin{aligned} \Gamma &= (\tau_1)^{-1} \frac{1}{T_l^{-1} \mu_l + T_v^{-1} \mu_v} \frac{\alpha_l \rho_l \alpha_v \rho_v}{\alpha_l \rho_l + \alpha_v \rho_v} (T_l^{-1} \mu_l - T_v^{-1} \mu_v) \\ \mathcal{A} &= (\tau_2)^{-1} \frac{\alpha_l \alpha_v}{P_l + P_v} (P_l - P_v) \\ \mathcal{B} &= (\tau_3)^{-1} \frac{\alpha_l \rho_l \alpha_v \rho_v}{\alpha_l \rho_l + \alpha_v \rho_v} (U_v - U_l) \\ \mathcal{C} &= (\tau_4)^{-1} \frac{\alpha_l \rho_l C_{V,l} \alpha_v \rho_v C_{V,v}}{\alpha_l \rho_l C_{V,l} + \alpha_v \rho_v C_{V,v}} (T_v - T_l) \end{aligned} \tag{5.11}$$

avec pour $\phi = l, v$,

$$\mu_\phi = -g_\phi + \left(\frac{(U_\phi - V_I)^2}{2} + \left(H_I - \frac{V_I^2}{2} \right) \right)$$

et l'enthalpie libre (ou enthalpie de Gibbs) g_ϕ qui s'écrit :

$$g_\phi = \left(e_\phi + \frac{P_\phi}{\rho_\phi} \right) - T_\phi s_\phi$$

La fermeture du terme H_I est la suivante:

$$H_I - \frac{V_I^2}{2} = 0$$

Ainsi, dans le cas où les vitesses sont équilibrées $U_l = U_v$, l'équilibre $\Gamma = 0$ est atteint si la relation $T_l^{-1} g_l - T_v^{-1} g_v = 0$ est vérifiée. Le même type d'équilibre a été obtenu dans [17] *dans le cadre isotherme*, c'est-à-dire pour $T_l = T_v$.

Le système est totalement fermé aux fréquences bornées positives τ_k^{-1} $k = 1,2,3,4$ près.

Il est communément admis que V_I doit correspondre à la vitesse de la phase diluée. Dans le cadre des écoulements diphasiques dans le circuit primaire, le choix $\delta = 0$ s'impose donc. Nous avons donc :

$$V_I = U_v, \quad H_I = \frac{U_v^2}{2} \quad \text{et} \quad P_I = P_l \tag{5.12}$$

Les notations H_I , V_I et P_I seront néanmoins conservées lorsque cela est possible.

Remarque. *Lorsque l'on considère les solutions régulières du système (5.1), les entropies physiques satisfont l'équation suivante :*

$$\partial_t (s_\phi) + U_\phi \partial_x (s_\phi) + \left[\left(\partial_{P_\phi} (s_\phi) \Big|_{\rho_\phi} \right) \left(\partial_{P_\phi} (e_\phi) \Big|_{\rho_\phi} \right)^{-1} \frac{(U_\phi - V_I)(P_I - P_\phi)}{\alpha_\phi \rho_\phi} \right] \partial_x (\alpha_\phi) = 0 \quad \phi = l, v \quad (5.13)$$

Avec les choix $\delta = 0$ et $\delta = 1$, les équations (5.13) deviennent simplement :

$$\partial_t (s_\phi) + U_\phi \partial_x (s_\phi) = 0 \quad \phi = l, v \quad (5.14)$$

Remarque. *Grâce aux fermetures du modèle à 7 équations, notamment l'hypothèse de champ linéairement dégénéré pour $\lambda = V_I$, on vérifie numériquement que les solutions approchées du système de convection pure, discrétisé à l'aide de deux schémas numériques distincts, convergent vers la même solution (voir [46]).*

5.3 Dérivation du modèle bi-fluide standard à partir du modèle bi-fluide à deux pressions

Cette section constitue à la fois un bref rappel sur le modèle bi-fluide standard et une présentation succincte d'une méthode employée pour obtenir des approximations numériques des solutions de ce modèle en utilisant le modèle bi-fluide à deux pressions présenté à la section précédente. Cette méthode est présentée en détail dans l'annexe C. Pour une présentation détaillée des modèles à une pression, le lecteur peut se référer à [56].

5.3.1 Description du modèle bi-fluide standard

Le modèle bi-fluide standard est un modèle à six équations qui suppose que les pressions phasiques et interfaciales sont en équilibre $P_l = P_v = P_I = P$. En reprenant les notations de la section précédente, le système d'équations est :

$$\begin{cases} \partial_t (\alpha_l \rho_l) + \partial_x (\alpha_l \rho_l U_l) = S_{2,l} \\ \partial_t (\alpha_l \rho_l U_l) + \partial_x (\alpha_l \rho_l U_l^2 + \alpha_l P) - P \partial_x (\alpha_l) = S_{3,l} \\ \partial_t (\alpha_l E_l) + \partial_x (\alpha_l U_l (E_l + P)) + P \partial_t (\alpha_l) = S_{4,l} \\ \partial_t (\alpha_v \rho_v) + \partial_x (\alpha_v \rho_v U_v) = S_{2,v} \\ \partial_t (\alpha_v \rho_v U_v) + \partial_x (\alpha_v \rho_v U_v^2 + \alpha_v P) - P \partial_x (\alpha_v) = S_{3,v} \\ \partial_t (\alpha_v E_v) + \partial_x (\alpha_v U_v (E_v + P)) + P \partial_t (\alpha_v) = S_{4,v} \end{cases} \quad (5.15)$$

avec l'énergie totale phasique:

$$E_\phi = \rho_\phi e_\phi(P, \rho_\phi) + \rho_\phi \frac{U_\phi^2}{2}, \quad \phi = v, l$$

où l'énergie interne s'écrit pour des gaz raides,

$$(\gamma_\phi - 1) \rho_\phi e_\phi = P + \gamma_\phi P_{\infty, \phi}, \quad \phi = v, l \quad (5.16)$$

Remarque. Ce modèle est connu comme n'étant que conditionnellement hyperbolique. Dans le cadre général les vecteurs de la matrice de convection ne sont pas connus. Cela limite considérablement le choix des schémas numériques envisageables pour la simulation numérique.

Le terme de transfert de masse $S_{2,\phi}$ est proportionnel à la fois à $\alpha_l \rho_l$ et à $\alpha_v \rho_v$, le lemme classique en annexe 4 du chapitre 4 peut donc être appliqué aux équations de masses partielles liquide et vapeur. Ceci assure la positivité des masses partielles $m_l = \alpha_l \rho_l$ et $m_v = \alpha_v \rho_v$.

Il est possible d'énoncer un principe du maximum pour le titre α_l en faisant quelques hypothèses sur la solution et en utilisant le résultat énoncé ci-dessus pour la positivité des masses partielles. On suppose que la solution est connue pour les variables vitesses $U_l(x, t)$ et $U_v(x, t)$ ainsi que pour les entropies $s_l(x, t)$ et $s_v(x, t)$. Le système (5.15) se résume alors aux deux équations sur les masses partielles et les seules inconnues restantes sont la pression P et le titre liquide α_l . Comme les vitesses phasiques sont connues, les équations sur les masses partielles définissent de façon implicite $m_l(x, t)$ et $m_v(x, t)$. On omettra dans la suite les arguments (x, t) sans perte de généralité. La relation sur les titres $\alpha_l + \alpha_v = 1$ se réécrit alors:

$$\frac{m_l}{\rho_l(P, s_l)} + \frac{m_v}{\rho_v(P, s_v)} = 1$$

On définit la fonction $\Pi \mapsto \mathcal{G}(\Pi)$ dont P est un pôle :

$$\mathcal{G}(\Pi) = \frac{m_l}{\rho_l(\Pi, s_l)} + \frac{m_v}{\rho_v(\Pi, s_v)} - 1 \quad (5.17)$$

et qui a pour domaine de définition $\Pi \in]\max(-P_{\infty, l}; -P_{\infty, v}); +\infty[$. Sa dérivée est :

$$\mathcal{G}'(\Pi) = -\frac{m_l}{(\rho_l(\Pi, s_l))^2} \partial_P(\rho_l)(\Pi, s_l) - \frac{m_v}{(\rho_v(\Pi, s_v))^2} \partial_P(\rho_v)(\Pi, s_v) \quad (5.18)$$

où pour le domaine en pression considéré, les dérivées $\partial_P(\rho_l)$ et $\partial_P(\rho_v)$ sont positives. On en déduit donc que :

$$\mathcal{G}'(\Pi) < 0$$

Or sur les bords du domaine de définition de \mathcal{G} on a :

$$\lim_{(\Pi \rightarrow \max(-P_{\infty, l}; -P_{\infty, v}))} \mathcal{G}(\Pi) = +\infty \quad \text{et} \quad \lim_{(\Pi \rightarrow +\infty)} \mathcal{G}(\Pi) = -1$$

Donc P est l'unique pôle de la fonction \mathcal{G} dans $]\max(-P_{\infty, l}; -P_{\infty, v}); +\infty[$. On en déduit grâce aux formules de $\rho_l(P_l, s_l)$ et $\rho_v(P_v, s_v)$ issues des définitions (5.5) que *les densités liquide et vapeur sont positives*. En utilisant le résultat de positivité sur les masses partielles on peut donc conclure que *les titres liquide et vapeur sont positifs* car $\alpha_\phi = m_\phi / \rho_\phi$.

5.3.2 Relaxation du modèle 7 équations en un modèle 6 équations

L'idée de cette méthode est de tirer avantage de la structure hyperbolique du modèle bi-fluide à deux pressions pour simuler le modèle bi-fluide standard. La méthode se décompose en deux étapes :

1. a) une étape de convection ;
b) une étape de prise en compte des termes sources physiques ;
2. une étape de relaxation instantanée où l'équilibre de pression est rétabli.

Remarque. *Dans la présentation ci-dessus, il a été choisi de traiter les termes sources physiques à l'aide d'une technique de pas fractionnaires. Si on avait choisi, par exemple, une méthode de dé-centrement de ces termes sources (voir chapitre 2), les étapes 1.a et 1.b serait confondues en une unique étape.*

La première étape consiste à appliquer au système (5.19) les schémas numériques classiquement utilisés pour simuler les systèmes hyperboliques sous forme non-conservative avec termes sources.

$$\left\{ \begin{array}{l} \partial_t(\alpha_l) + V_I \partial_x(\alpha_l) = 0 \\ \partial_t(\alpha_l \rho_l) + \partial_x(\alpha_l \rho_l U_l) = S_{2,l} \\ \partial_t(\alpha_l \rho_l U_l) + \partial_x(\alpha_l \rho_l U_l^2 + \alpha_l P_l) - P_I \partial_x(\alpha_l) = S_{3,l} \\ \partial_t(\alpha_l E_l) + \partial_x(\alpha_l U_l (E_l + P_l)) = S_{4,l} \\ \partial_t(\alpha_v \rho_v) + \partial_x(\alpha_v \rho_v U_v) = S_{2,v} \\ \partial_t(\alpha_v \rho_v U_v) + \partial_x(\alpha_v \rho_v U_v^2 + \alpha_v P_v) - P_I \partial_x(\alpha_v) = S_{3,v} \\ \partial_t(\alpha_v E_v) + \partial_x(\alpha_v U_v (E_v + P_v)) = S_{4,v} \end{array} \right. \quad (5.19)$$

A l'issue de cette étape on obtient des approximations des variables notées $(\tilde{\alpha}_l, \tilde{\rho}_l, \tilde{U}_l, \tilde{P}_l, \tilde{\rho}_v, \tilde{U}_v, \tilde{P}_v)$ où les pressions phasiques obtenues ne sont pas nécessairement équilibrées, on a $\tilde{P}_l \neq \tilde{P}_v$. La deuxième

étape est basée sur la résolution du système :

$$\begin{cases} \partial_t (\alpha_l) = \mathcal{A} \\ \partial_t (\alpha_l \rho_l) = 0 \\ \partial_t (\alpha_l \rho_l U_l) = 0 \\ \partial_t (\alpha_l E_l) + P \partial_t (\alpha_l) = 0 \\ \partial_t (\alpha_v \rho_v) = 0 \\ \partial_t (\alpha_v \rho_v U_v) = 0 \\ \partial_t (\alpha_v E_v) + P \partial_t (\alpha_v) = 0 \end{cases} \quad (5.20)$$

où le temps de relaxation du terme source \mathcal{A} est formellement nul, $\tau_1 = 0$. La première équation du système (5.20) s'écrit donc $P_l = P_v = P$, ce qui grâce aux lois de fermeture donne $P_l = P$. Ce système est discrétisé de manière implicite vis-à-vis de la pression :

$$\begin{cases} P_l^{n+1} = P_v^{n+1} = P^{n+1} \\ (\alpha_l \rho_l)^{n+1} = (\tilde{\alpha}_l \tilde{\rho}_l) \\ (\alpha_l \rho_l U_l)^{n+1} = (\tilde{\alpha}_l \tilde{\rho}_l \tilde{U}_l) \\ \left((\alpha_l \rho_l)^{n+1} e_l(P^{n+1}, \rho_l^{n+1}) - \tilde{\alpha}_l \tilde{\rho}_l e_l(\tilde{P}_l, \tilde{\rho}_l) \right) + \left(\left(\frac{\alpha_l \rho_l U_l^2}{2} \right)^{n+1} - \frac{\tilde{\alpha}_l \tilde{\rho}_l \tilde{U}_l^2}{2} \right) = P^{n+1} (\tilde{\alpha}_l - \alpha_l^{n+1}) \\ (\alpha_v \rho_v)^{n+1} = (\tilde{\alpha}_v \tilde{\rho}_v) \\ (\alpha_v \rho_v U_v)^{n+1} = (\tilde{\alpha}_v \tilde{\rho}_v \tilde{U}_v) \\ \left((\alpha_v \rho_v)^{n+1} e_v(P^{n+1}, \rho_v^{n+1}) - \tilde{\alpha}_v \tilde{\rho}_v e_v(\tilde{P}_v, \tilde{\rho}_v) \right) + \left(\left(\frac{\alpha_v \rho_v U_v^2}{2} \right)^{n+1} - \frac{\tilde{\alpha}_v \tilde{\rho}_v \tilde{U}_v^2}{2} \right) = P^{n+1} (\tilde{\alpha}_v - \alpha_v^{n+1}) \end{cases} \quad (5.21)$$

Pour deux gaz raides, la mise à jour des titres liquide et vapeur se fait par les formules :

$$\alpha_\phi^{n+1} = \frac{\tilde{\alpha}_\phi}{\gamma_\phi} \left((\gamma_\phi - 1) + \frac{\tilde{P}_\phi + P_{\infty, \phi}}{P^{n+1} + P_{\infty, \phi}} \right), \quad \phi = l, v \quad (5.22)$$

On suppose sans perte de généralité que $P_{\infty, v} \leq P_{\infty, l}$. On suppose de plus que les titres $\tilde{\alpha}_v$ et $\tilde{\alpha}_l$ sont positifs et que le vide n'est apparu dans aucune des phases, c'est-à-dire que l'on a $\tilde{P}_v + P_{\infty, v} > 0$ et $\tilde{P}_l + P_{\infty, l} > 0$. La nouvelle pression déduite de l'unique racine positive du polynôme du second degré en $(P^{n+1} + P_{\infty, v})$:

$$C_2 (P^{n+1} + P_{\infty, v})^2 + C_1 (P^{n+1} + P_{\infty, v}) + C_0$$

dont les coefficients sont,

$$\begin{cases} C_2 = \frac{\tilde{\alpha}_l}{\gamma_l} + \frac{\tilde{\alpha}_v}{\gamma_v} > 0 \\ C_1 = -\frac{\tilde{\alpha}_l}{\gamma_l} (\tilde{P}_l + P_{\infty, v}) - \frac{\tilde{\alpha}_v}{\gamma_v} (\tilde{P}_v + P_{\infty, l}) \\ C_0 = -\frac{\tilde{\alpha}_v}{\gamma_v} (P_{\infty, l} - P_{\infty, v}) (\tilde{P}_v + P_{\infty, v}) < 0 \end{cases} \quad (5.23)$$

est donc :

$$P^{n+1} + P_{\infty, v} = \frac{-C_1 + \sqrt{C_1^2 - 4C_2 C_0}}{2C_2} \quad (5.24)$$

Elle garantit l'admissibilité physique de P^{n+1} et de α_l^{n+1} .

De plus si on avait initialement un équilibre des pressions phasiques $\tilde{P}_v = \tilde{P}_l$, la formule (5.24) nous assure la conservation de cet équilibre $P^{n+1} = \tilde{P}_v = \tilde{P}_l$ à condition que $P_{\infty,l} = P_{\infty,v}$.

Propriété 1. Soit un état initial de l'étape de relaxation instantanée tel que les pressions phasiques sont en équilibre. L'équilibre en pression est conservé par l'étape de relaxation instantanée, issu de la formule (5.24), si et seulement si les lois d'état phasiques vérifient $P_{\infty,l} = P_{\infty,v}$. Autrement dit on a :

$$P^{n+1} = \tilde{P}_l = \tilde{P}_v \iff P_{\infty,l} = P_{\infty,v}$$

Remarque. Ces résultats sont une généralisation de ceux obtenus dans le cadre de lois d'état de type gaz parfaits $P_{\infty,l} = P_{\infty,v} = 0$ (voir annexe C). Pour deux lois de type gaz parfait, la mise à jour des pressions phasiques et des titres liquide et vapeur se fait en utilisant les relations :

$$P^{n+1} = \frac{\tilde{\alpha}_l \gamma_v \tilde{P}_l + \tilde{\alpha}_v \gamma_l \tilde{P}_v}{\tilde{\alpha}_l \gamma_v + \tilde{\alpha}_v \gamma_l} \quad (5.25)$$

$$\alpha_\phi^{n+1} = \frac{\tilde{\alpha}_\phi}{\gamma_\phi} \left((\gamma_\phi - 1) + \frac{\tilde{P}_\phi}{P^{n+1}} \right), \quad \phi = l, v \quad (5.26)$$

Si les pressions \tilde{P}_l , \tilde{P}_v et les titres α_l , α_v sont positifs, les nouvelles valeurs de la pression et des titres liquide et vapeur sont positifs.

5.4 Dérivation du modèle homogène relaxé (HRM) à partir du modèle bi-fluide à deux pressions

Le modèle homogène relaxé, ou modèle HRM, est un modèle largement utilisé pour la simulation des écoulements diphasiques dans le domaine nucléaire. Il est construit sur un système de quatre équations qui sont en partie basées sur des grandeurs physiques moyennes. Celles-ci sont la densité du mélange ρ et la vitesse moyenne du mélange U . Les deux autres grandeurs sont la pression P du mélange et le titre de la phase liquide α . Dans le cas de modèles où les deux phases ont la même vitesse, la partie convective du système d'équations est de la forme :

$$\begin{cases} \partial_t(\rho\alpha) + \partial_x(\rho\alpha U) = 0 \\ \partial_t(\rho) + \partial_x(\rho U) = 0 \\ \partial_t(\rho U) + \partial_x(\rho U^2 + P) = 0 \\ \partial_t(E) + \partial_x(U(E + P)) = 0 \end{cases} \quad (5.27)$$

avec l'énergie totale $E = \rho e(P, \rho, \alpha) + \rho U^2/2$.

Dans cette section, on utilise une méthode de relaxation pour simuler un modèle HRM à partir du modèle bi-fluide à deux pressions (5.1) précédemment présenté. Cette méthode comprend deux étapes. Une première étape prend en compte les phénomènes physiques, à savoir la convection et les termes sources physiques Γ , $V_I\Gamma$ et $H_I\Gamma$. La deuxième étape est l'étape de relaxation : on pose $\tau_2 = \tau_3 = \tau_4 = 0$. Le but de cette dernière étape est de projeter la solution sur un sous-ensemble de solutions pour lesquelles on a équilibre des vitesses, pressions et températures physiques.

5.4.1 Etape de convection et de prise en compte des termes source physiques

Cette première étape consiste à simuler le système (5.28) qui est obtenu en posant $\mathcal{A} = 0$, $\mathcal{B} = 0$ et $\mathcal{C} = 0$ dans le système (5.1).

$$\begin{cases} \partial_t(\alpha_l) + V_I\partial_x(\alpha_l) = 0 \\ \partial_t(\alpha_l\rho_l) + \partial_x(\alpha_l\rho_l U_l) = \Gamma \\ \partial_t(\alpha_l\rho_l U_l) + \partial_x(\alpha_l\rho_l U_l^2 + \alpha_l P_l) - P_I\partial_x(\alpha_l) = V_I\Gamma \\ \partial_t(\alpha_l E_l) + \partial_x(\alpha_l U_l(E_l + P_l)) - P_I V_I\partial_x(\alpha_l) = H_I\Gamma \\ \partial_t(\alpha_v\rho_v) + \partial_x(\alpha_v\rho_v U_v) = -\Gamma \\ \partial_t(\alpha_v\rho_v U_v) + \partial_x(\alpha_v\rho_v U_v^2 + \alpha_v P_v) - P_I\partial_x(\alpha_v) = -V_I\Gamma \\ \partial_t(\alpha_v E_v) + \partial_x(\alpha_v U_v(E_v + P_v)) - P_I V_I\partial_x(\alpha_v) = -H_I\Gamma \end{cases} \quad (5.28)$$

En général, à l'issue de cette étape, les vitesses phasiques, pressions phasiques et températures phasiques ne sont pas équilibrées.

5.4.2 Etape de relaxation instantanée en pression, vitesse et température

Pour cette deuxième étape, Γ est considéré comme étant nul, ainsi que, formellement, les temps de relaxation τ_2 , τ_3 et τ_4 . Le système correspondant est :

$$\begin{cases} P_l = P_v \\ U_l = U_v \\ T_l = T_v \\ \partial_t (\alpha_l \rho_l) = 0 \\ \partial_t (\alpha_v \rho_v) = 0 \\ \partial_t (\alpha_l \rho_l U_l + \alpha_v \rho_v U_v) = 0 \\ \partial_t (\alpha_l E_l + \alpha_v E_v) = 0 \end{cases} \quad (5.29)$$

Il reste à préciser la façon dont on discrétise ce système. On notera par un tilde les variables obtenues à la fin de la première étape, les grandeurs calculées à la fin de l'étape de relaxation seront indicées par $n+1$.

Le système (5.29) est discrétisé de la façon suivante :

$$\begin{cases} P_l^{n+1} = P_v^{n+1} = P^{n+1} \\ U_l^{n+1} = U_v^{n+1} = U^{n+1} \\ T_l(P_l^{n+1}, \rho_l^{n+1}) = T_v(P_v^{n+1}, \rho_v^{n+1}) \\ (\alpha_l \rho_l)^{n+1} = \tilde{\alpha}_l \tilde{\rho}_l \\ (\alpha_v \rho_v)^{n+1} = \tilde{\alpha}_v \tilde{\rho}_v \\ (\alpha_l \rho_l U_l + \alpha_v \rho_v U_v)^{n+1} = \tilde{\alpha}_l \tilde{\rho}_l \tilde{U}_l + \tilde{\alpha}_v \tilde{\rho}_v \tilde{U}_v \\ (\alpha_l E_l + \alpha_v E_v)^{n+1} = \tilde{\alpha}_l \tilde{E}_l + \tilde{\alpha}_v \tilde{E}_v \end{cases} \quad (5.30)$$

L'équation de conservation de l'impulsion totale fournit la définition de la nouvelle valeur de la vitesse U^{n+1} qui est indépendante de la forme exacte de la thermodynamique :

$$U^{n+1} = \frac{\tilde{\alpha}_l \tilde{\rho}_l \tilde{U}_l + \tilde{\alpha}_v \tilde{\rho}_v \tilde{U}_v}{\tilde{\alpha}_l \tilde{\rho}_l + \tilde{\alpha}_v \tilde{\rho}_v} \quad (5.31)$$

Remarque. La vitesse après relaxation instantanée étant une moyenne des vitesses phasiques avant relaxation pondérée par les masses partielles, on a la relation triviale : $\tilde{U}_l = \tilde{U}_v \implies U^{n+1} = \tilde{U}_l = \tilde{U}_v$

En utilisant les quatrième et cinquième équations, la troisième équation et la dernière équation peuvent être réécrites uniquement en fonction de la pression P^{n+1} et du titre liquide α_l^{n+1} , formant ainsi le système non-linéaire de deux équations à deux inconnues suivant :

$$\begin{cases} \frac{P^{n+1} + P_{\infty,l}}{C_{V,l}(\gamma_l - 1) \tilde{\alpha}_l \tilde{\rho}_l} \alpha_l^{n+1} - \frac{P^{n+1} + P_{\infty,v}}{C_{V,v}(\gamma_v - 1) \tilde{\alpha}_v \tilde{\rho}_v} (1 - \alpha_l^{n+1}) = 0 \\ \frac{P^{n+1} + \gamma_l P_{\infty,l}}{(\gamma_l - 1)} \alpha_l^{n+1} + \frac{P^{n+1} + \gamma_v P_{\infty,v}}{(\gamma_v - 1)} (1 - \alpha_l^{n+1}) = \tilde{\epsilon} \end{cases} \quad (5.32)$$

où on a posé :

$$\tilde{\epsilon} = \tilde{\alpha}_l \tilde{\rho}_l e_l(\tilde{P}_l, \tilde{\rho}_l) + \tilde{\alpha}_v \tilde{\rho}_v e_v(\tilde{P}_v, \tilde{\rho}_v) + \frac{1}{2} \frac{\tilde{\alpha}_l \tilde{\rho}_l \tilde{\alpha}_v \tilde{\rho}_v}{\tilde{\alpha}_l \tilde{\rho}_l + \tilde{\alpha}_v \tilde{\rho}_v} (\tilde{U}_l - \tilde{U}_v)^2$$

Pourvu que le vide n'apparaisse dans aucune des deux phases, autrement dit que la condition (5.33) soit remplie, la première équation du système (5.32) nous assure la positivité des titres α_l^{n+1} et α_v^{n+1} .

$$P^{n+1} + \min(P_{\infty,l}; P_{\infty,v}) > 0 \quad (\iff P^{n+1} > \max(-P_{\infty,l}; -P_{\infty,v})) \quad (5.33)$$

On fait l'hypothèse que les coefficients des lois d'état des deux phases sont telles que :

$$P_{\infty,l} \geq P_{\infty,v} \quad (5.34)$$

Le système (5.32) fournit l'équation résolvante en pression suivante :

$$D_2(P^{n+1} + P_{\infty,v})^2 + D_1(P^{n+1} + P_{\infty,v}) + D_0 = 0 \quad (5.35)$$

avec les coefficients suivants :

$$\begin{cases} D_2 = C_{V,l}\tilde{\alpha}_l\tilde{\rho}_l + C_{V,v}\tilde{\alpha}_v\tilde{\rho}_v \\ D_1 = C_{V,l}\tilde{\alpha}_l\tilde{\rho}_l(P_{\infty,l} - P_{\infty,v} + (\gamma_l - 1)(P_{\infty,l} - \tilde{\epsilon})) \\ \quad + C_{V,v}\tilde{\alpha}_v\tilde{\rho}_v(P_{\infty,l} - P_{\infty,v} + (\gamma_v - 1)(P_{\infty,v} - \tilde{\epsilon})) \\ D_0 = C_{V,v}\tilde{\alpha}_v\tilde{\rho}_v(\gamma_v - 1)(P_{\infty,l} - P_{\infty,v})(P_{\infty,v} - \tilde{\epsilon}) \end{cases} \quad (5.36)$$

Grâce à l'hypothèse (5.34), le coefficient D_0 est négatif. Le polynôme possède une unique solution pression $(P^{n+1} + P_{\infty,v})$ positive :

$$P^{n+1} + P_{\infty,v} = \frac{-D_1 + \sqrt{D_1^2 - 4D_2D_0}}{2D_2} \quad (5.37)$$

La condition (5.33) est alors trivialement vérifiée et les nouveaux titres vapeur et liquide sont positifs.

On en déduit alors la formule des autres variables du modèle à sept équations :

$$\begin{cases} \alpha_l^{n+1} = \frac{(P^{n+1} + P_{\infty,v})\xi_v}{(P^{n+1} + P_{\infty,l})\xi_l + (P^{n+1} + P_{\infty,v})\xi_v} \\ \rho_l^{n+1} = \frac{\tilde{\alpha}_l\tilde{\rho}_l}{\alpha_l^{n+1}} \\ \rho_v^{n+1} = \frac{\tilde{\alpha}_v\tilde{\rho}_v}{1 - \alpha_l^{n+1}} \end{cases} \quad (5.38)$$

avec $\xi_v^{-1} = C_{V,v}\tilde{\alpha}_v\tilde{\rho}_v(\gamma_v - 1)$ et $\xi_l^{-1} = C_{V,l}\tilde{\alpha}_l\tilde{\rho}_l(\gamma_l - 1)$. Cette formule permet de retrouver que α_l^{n+1} reste entre 0 et 1.

Finalement les sept variables physiques du modèle bi-fluide à deux pressions sont mises à jour suivant les formules :

$$\begin{cases} \alpha_l^{n+1} = \left(1 + \left(\frac{P^{n+1} + P_{\infty,l}}{P^{n+1} + P_{\infty,v}}\right) \frac{C_{V,v}\tilde{\alpha}_v\tilde{\rho}_v(\gamma_v - 1)}{C_{V,l}\tilde{\alpha}_l\tilde{\rho}_l(\gamma_l - 1)}\right)^{-1} \\ \rho_l^{n+1} = \frac{\tilde{\alpha}_l\tilde{\rho}_l}{\alpha_l^{n+1}} \\ U_l^{n+1} = U^{n+1} \\ P_l^{n+1} = P^{n+1} \\ \rho_v^{n+1} = \frac{\tilde{\alpha}_v\tilde{\rho}_v}{1 - \alpha_l^{n+1}} \\ U_v^{n+1} = U^{n+1} \\ P_v^{n+1} = P^{n+1} \end{cases} \quad (5.39)$$

De façon classique pour les modèles HRM, on définit la densité ρ du mélange comme étant la somme des masses partielles : $\rho = \alpha_l\rho_l + \alpha_v\rho_v$. Celle-ci vaut donc à la fin de l'étape de relaxation instantanée :

$$\rho^{n+1} = \tilde{\alpha}_l\tilde{\rho}_l + \tilde{\alpha}_v\tilde{\rho}_v$$

De même le titre masse liquide C est défini par la relation $C\rho = \alpha_l\rho_l$ d'où la nouvelle valeur du titre masse liquide C^{n+1} après relaxation :

$$C^{n+1} = \frac{\tilde{\alpha}_l\tilde{\rho}_l}{\tilde{\alpha}_l\tilde{\rho}_l + \tilde{\alpha}_v\tilde{\rho}_v}$$

Remarque. Avec ces définitions de ρ et C on a :

$$\rho^{n+1} = \tilde{\rho} \quad \text{et} \quad C^{n+1} = \tilde{C}$$

Les quatre variables du modèle HRM sont donc explicitement connues celles-ci sont :

$$\begin{cases} C^{n+1} = \frac{\tilde{\alpha}_l\tilde{\rho}_l}{\tilde{\alpha}_l\tilde{\rho}_l + \tilde{\alpha}_v\tilde{\rho}_v} \\ \rho^{n+1} = \tilde{\alpha}_l\tilde{\rho}_l + \tilde{\alpha}_v\tilde{\rho}_v \\ U^{n+1} \\ P^{n+1} \end{cases} \quad (5.40)$$

Remarque. Dans le cadre d'une prise en compte numérique des termes sources par méthode à pas fractionnaires, l'interversion de l'étape de relaxation instantanée et de l'étape de relaxation physique n'est pas possible. En effet, la relaxation physique ne permet pas de maintenir à la fois l'équilibre des pressions et l'équilibre des températures.

Les formules de α_l^{n+1} , ρ_l^{n+1} , U_l^{n+1} , P_l^{n+1} , ρ_v^{n+1} , U_v^{n+1} et P_v^{n+1} permettent donc de retrouver un état pour lequel les vitesses, pressions et températures sont égales au sein des deux phases. Il reste à vérifier si certains équilibres sont conservés par cette projection.

Propriété 2. Si l'état initial de l'étape de relaxation instantanée est tel que les vitesses et températures phasiques sont en équilibre, alors l'état calculé grâce aux formules (5.36), (5.37) et (5.39) est tel que les mêmes équilibres sont conservés. Plus précisément on a :

$$\tilde{T}_l = \tilde{T}_v = \tilde{T} \quad \text{et} \quad \tilde{U}_l = \tilde{U}_v = \tilde{U} \quad \implies \quad T^{n+1} = \tilde{T} \quad \text{et} \quad U^{n+1} = \tilde{U}$$

Propriété 3. Soit un état initial de l'étape de relaxation instantanée tel que les pressions phasiques sont en équilibre. L'équilibre en pression est conservé par l'étape de relaxation instantanée si et seulement si :

- (i) les vitesses phasiques sont équilibrées $\tilde{U}_l = \tilde{U}_v$
- (ii) les lois d'état phasiques sont identiques, c'est-à-dire que l'on a,

$$\gamma_l = \gamma_v \quad \text{et} \quad P_{\infty,l} = P_{\infty,v}$$

Remarque. Dans le cadre de la propriété 3, les coefficients thermodynamiques $C_{V,l}$ et $C_{V,v}$ peuvent être choisis indépendamment l'un de l'autre.

5.5 Une méthode de couplage des modèles bi-fluide standard et HRM

Dans cette section on se propose de coupler les modèles bi-fluide standard et HRM présentés ci-dessus. Le couplage s'effectuera grâce à un modèle père basé sur le modèle bi-fluide à deux pressions dont on a vu qu'il permettait d'obtenir par une méthode de relaxation à la fois le modèle bi-fluide standard et le modèle HRM. Ce modèle d'interface permettra de calculer, via la résolution d'un problème de Riemann, les flux numériques qui serviront de conditions aux limites pour les codes droit et gauche.

On supposera maintenant que le code de gauche (i.e. pour les x négatifs) est basé sur le modèle bi-fluide standard et que le code de droite (i.e. pour les x positifs) simule quant à lui le modèle HRM. L'interface de couplage se situe donc en $x = 0$.

5.5.1 Le modèle d'interface

On introduit une variable Y dépendant de x et t et dont la donnée initiale, notée Y_0 , est telle que $Y_0(x) = Y(x,0) = 0$ pour $x < 0$ et $Y_0(x) = Y(x,0) = 1$ pour $x > 0$. Cette variable, appelée variable "couleur" ou "domaine", est régie par l'équation aux dérivées partielles :

$$\partial_t(Y) = 0$$

Le modèle d'interface est alors :

$$\left\{ \begin{array}{l} \partial_t(Y) = 0 \\ \partial_t(\alpha_l) + V_I \partial_x(\alpha_l) = \mathcal{A} \\ \partial_t(\alpha_l \rho_l) + \partial_x(\alpha_l \rho_l U_l) = \Gamma \\ \partial_t(\alpha_l \rho_l U_l) + \partial_x(\alpha_l \rho_l U_l^2 + \alpha_l P_l) - P_I \partial_x(\alpha_l) = \Psi_{3,l}(Y) \\ \partial_t(\alpha_l E_l) + \partial_x(\alpha_l U_l (E_l + P_l)) + P_I \partial_t(\alpha_l) = \Psi_{4,l}(Y) \\ \partial_t(\alpha_v \rho_v) + \partial_x(\alpha_v \rho_v U_v) = -\Gamma \\ \partial_t(\alpha_v \rho_v U_v) + \partial_x(\alpha_v \rho_v U_v^2 + \alpha_v P_v) - P_I \partial_x(\alpha_v) = -\Psi_{3,l}(Y) \\ \partial_t(\alpha_v E_v) + \partial_x(\alpha_v U_v (E_v + P_v)) + P_I \partial_t(\alpha_v) = -\Psi_{4,l}(Y) \end{array} \right. \quad (5.41)$$

où le couple (V_I, P_I) est celui de la section 2. Les définitions des énergies phasiques totales ou des énergies phasiques internes sont identiques à celles du modèle bi-fluide à deux pressions de la section 2 (voir équations (5.2) et (5.3)).

Les termes sources $\Psi_{3,l}$ et $\Psi_{4,l}$ s'écrivent de manière formelle :

$$\Psi_{3,l} = (1 - Y)^{-1} \mathcal{B} + V_I \Gamma \quad (5.42)$$

$$\Psi_{4,l} = (1 - Y)^{-1} (\mathcal{C} + V_I \mathcal{B}) + H_I \Gamma \quad (5.43)$$

Dans le cadre de la simulation des modèles bi-fluide standard et HRM, la constante de temps τ_2 est toujours nulle. Ainsi, si la variable Y est nulle on retrouve formellement le système (5.15) permettant la simulation du modèle bi-fluide standard et si Y est égale à 1 on retrouve le système permettant la simulation du modèle HRM.

A la différence du cas de couplage du chapitre précédent, la variable Y est transparente vis-à-vis des lois d'état, ce sont celles du modèle père pour les deux modèles. L'équation portant sur Y pourrait être choisie de la forme

$$\partial_t(Y) + \mathcal{U}\partial_x(Y) = \theta(Y_0 - Y)$$

où la valeur propre \mathcal{U} correspond à un champ linéairement dégénéré. Le cas $\mathcal{U} = 0$ et $\theta = 0$ est ici naturel car la structure propre du système (5.41) est indépendante de la variable Y . L'introduction du champ stationnaire associé à Y (cas $\mathcal{U} = 0$ et $\theta = 0$) ne sera donc pas à l'origine de phénomène de résonance. On aurait tout aussi bien pu envisager le choix $\mathcal{U} = V_I$ et $\theta = +\infty$. Une remarque à ce propos sera faite ultérieurement.

5.5.2 Le schéma de calcul

Le modèle d'interface décrit ci-dessus permet de simuler le modèle HRM ainsi que le modèle bi-fluide standard. Le couplage des deux modèles est quant à lui assuré par la partie convective du système (5.41). Le traitement des termes sources est effectué séparément de la convection en utilisant une technique de pas fractionnaires.

Les techniques utilisées sont de type Volumes Finis. A chaque cellule i du domaine discrétisé est attachée la valeur moyenne du vecteur $W = (Y, \alpha_l, \alpha_l \rho_l, \alpha_l \rho_l U_l, \alpha_l \rho_l E_l, \alpha_v, \alpha_v \rho_v, \alpha_v \rho_v U_v, \alpha_v \rho_v E_v)^\top$. L'initialisation des données est telle que $(P_l)_i = (P_v)_i$ si la cellule i est dans le domaine du modèle standard bi-fluide (i.e. si $Y_i=0$ ou encore si $x < 0$), et elle est telle que $(P_l)_i = (P_v)_i$, $(U_l)_i = (U_v)_i$ et $(T_l)_i = (T_v)_i$ si la cellule i se trouve dans le domaine correspondant au modèle HRM (i.e. si $Y_i=1$ ou encore si $x > 0$).

Le schéma de calcul des approximations des modèles HRM et bi-fluide standard et de leur couplage comporte ainsi trois étapes.

– Etape de convection:

La partie convective du système (5.41) est discrétisée en utilisant un schéma de type Rusanov (voir sous-section B.1) ou de type VFRoe-ncv (voir sous-section B.2). Lors de cette étape il n'est fait aucune distinction entre les modèles. La particularité du calcul au niveau de l'interface de couplage vient du fait que les données de droite (resp. gauche) alimentant les flux numériques sont équilibrées en vitesse, pression et température (resp. équilibrées en pression).

– Termes sources physiques:

La prise en compte des termes sources physiques est réalisée par des méthodes d'intégration semi-analytiques ou analytiques. Celles-ci sont détaillées en annexe 2.

– Relaxation instantanée:

Les formules permettant de calculer les états relaxés sont celles obtenues dans la section 3 pour le modèle bi-fluide standard et dans la section 4 pour le modèle HRM.

Même si le prototype développé est bi-dimensionnel, on se restreint pour la présentation au cas d'un maillage uniforme mono-dimensionnel.

Utilisation d'un schéma de Rusanov

Une première façon de calculer les flux de couplage consiste à utiliser un schéma de type Rusanov adapté au cas de systèmes d'équations écrits sous forme non-conservative.

Soit un système d'équations portant sur la variable W et écrit sous la forme non-conservative suivante :

$$\partial_t(W) + \partial_x(F(W)) + A(W)\partial_x(G(W)) = 0 \quad (5.44)$$

Un schéma numérique explicite de type volumes finis permettant la simulation de ce système s'écrit pour la cellule i :

$$\begin{aligned} \Delta x(W_i^{n+1} - W_i^n) + \Delta t \left((F^{Rus})_{i+1/2}^n - (F^{Rus})_{i-1/2}^n \right) \\ + \frac{1}{2}\Delta t A(W_i^n) (G(W_{i+1}^n) - G(W_{i-1}^n)) = 0 \end{aligned} \quad (5.45)$$

Le flux numérique $(F^{Rus})_{i+1/2}^n$ correspond au flux numérique de Rusanov classique calculé à l'interface entre la cellule i et la cellule $i+1$:

$$(F^{Rus})_{i+1/2}^n = \frac{F(W_{i+1}^n) + F(W_i^n)}{2} - \max(S_i^+, S_{i+1}^+) \frac{W_{i+1}^n - W_i^n}{2}$$

La grandeur S_i^+ est le rayon spectral de la matrice $(\partial_W(F(W)) + A(W)\partial_W(G(W)))$ dans la cellule i . Le pas de temps Δt est calculé en utilisant la condition CFL classique,

$$\Delta t = \min_i \left(\frac{CFL \times \Delta x}{S_i^+} \right)$$

On reconnaît dans la formule (5.45) l'expression de la dérivée première centrée sur la cellule i du terme convectif non-conservatif.

Utilisation d'un schéma VFRoe-ncv en variables $Q = (Y, \alpha_l, s_l, U_l, P_l, s_v, U_v, P_v)^\top$

Un schéma numérique explicite de type volumes finis permettant la simulation du système (5.44) s'écrit pour la cellule i :

$$\begin{aligned} \Delta x(W_i^{n+1} - W_i^n) + \Delta t \left((F^{VFRoe})_{i+1/2}^n - (F^{VFRoe})_{i-1/2}^n \right) \\ + \Delta t A \left(\frac{W_{i+1/2}^{*,n} + W_{i-1/2}^{*,n}}{2} \right) \left(G(W_{i+1/2}^{*,n}) - G(W_{i-1/2}^{*,n}) \right) = 0 \end{aligned} \quad (5.46)$$

où $W_{i+1/2}^{*,n} = W(Q_{i+1/2}^{*,n})$ et où $Q_{i+1/2}^{*,n}$ correspond à la solution en $x/t = 0$ du problème de Riemann linéaire (5.47) :

$$\partial_t(Q) + J(\bar{Q})\partial_x(Q) = 0, \quad Q(x, t = 0) = \begin{cases} Q_i & \text{si } x < 0 \\ Q_{i+1} & \text{si } x > 0 \end{cases} \quad (5.47)$$

La résolution de (5.47) ainsi que les définitions de J et \bar{Q} sont données dans l'annexe 1.

Remarques

- Les deux schémas numériques ci-dessus peuvent également être transposés au cadre multi-dimensionnel. L'utilisation du schéma de Godunov approché (ou exact) présente l'avantage pratique d'une extension simple au cadre multi-dimensionnel, ce qui ne serait pas le cas avec une linéarisée de Roe (calcul de la structure propre).
- Valeurs de V_I alternatives :
Au vu de l'annexe 1, on constate rapidement que le choix d'une valeur de V_I non nulle mais associée à un champ linéairement dégénéré ne modifie pas la structure d'onde associée aux variables $\alpha_l, s_l, U_l, P_l, s_v, U_v$ et P_v .

- Il serait intéressant de comparer la technique de relaxation instantanée utilisée ici avec une approche privilégiant la convergence vers un état d'équilibre à chaque pas de temps telle qu'utilisée dans [46], même si celle-ci est plus coûteuse en terme de CPU.

5.6 Résultats numériques en l'absence de transfert de masse

5.6.1 Cas test bi-dimensionnel d'écoulement tangent à l'interface de couplage

Les conditions initiales sont choisies de façon à avoir un équilibre initial en pression, vitesse et température. Les lois d'état phasiques sont des lois de type gaz parfaits avec les paramètres :

$$\gamma_l = \gamma_v = 1.24 \quad \text{et} \quad P_{\infty,l} = P_{\infty,v} = 0$$

$$C_{V,l} = 3036 \quad \text{et} \quad C_{V,v} = 31680$$

Le seul terme source physique considéré est la traînée dont le temps caractéristique est supposé constant et égal à :

$$\tau_3 = 10^{-4}$$

On néglige dans ce cas le transfert de masse $(\tau_1)^{-1} = 0$ et le transfert d'énergie $(\tau_4)^{-1} = 0$. Le domaine de calcul est le carré de côté 2 dont le coin inférieur gauche est situé à l'origine. Le maillage est régulier, uniforme et composé de 60×60 cellules. La CFL est fixée à 0.5.

L'objectif est ici à la fois de réaliser un calcul bi-dimensionnel sur maillage grossier, et d'évaluer la pollution associée à la présence d'une interface mince entre les deux codes, lorsque l'écoulement principal est tangent à l'interface. Ce cas test est donc complémentaire des tests suivants.

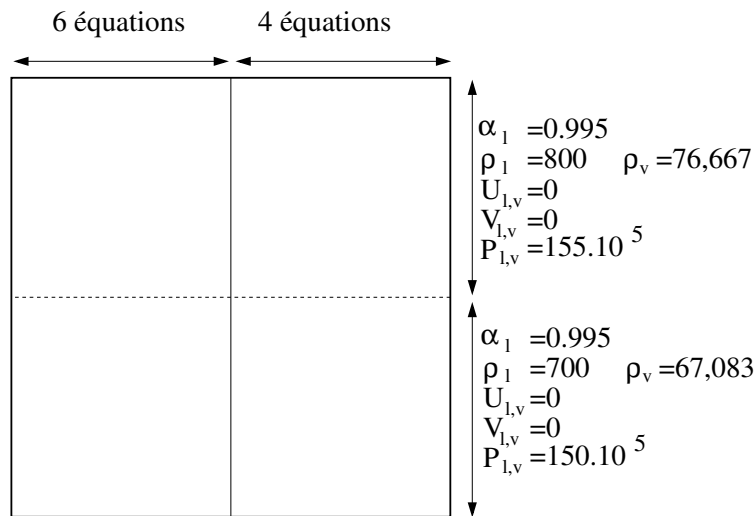


FIG. 5.1 – Configuration et conditions initiales

Les grandeurs post-traitées sont les grandeurs moyennes (densité de mélange, vitesse de mélange, pression du mélange), le pourcentage de l'écart relatif du titre masse par rapport à 0.999518 (titre masse liquide d'initialisation) et la vitesse relative. Pour toute variable, les profils dans le cas d'une simulation d'un seul modèle sur l'ensemble du domaine sont uniformes selon l'axe x , dans la mesure où le maillage est structuré orthogonal. Dans le cas couplé qui est présenté, on attend par contre un effet de distorsion lié à une représentation distincte de la vitesse relative de part et d'autre de l'interface de couplage (elle est structurellement nulle du côté correspondant au modèle HRM). Les approximations obtenues sur ce maillage de taille industrielle montrent que les profils des grandeurs

caractéristiques du mélange sont en fait uniformes selon x , à l'échelle de représentation des résultats. De fait, la vitesse de mélange (voir figures (5.5) et (5.4)) est pratiquement identique à la vitesse de la phase liquide, alors que la vitesse relative est du même ordre de grandeur que cette dernière (voir figures (5.7) et (5.6)). Si on ne connaissait pas la position de l'interface, seul le tracé de la vitesse relative permettrait de repérer celle-ci pour ce cas test. Il faut toutefois garder à l'esprit le fait que l'utilisation concomitante de la technique de relaxation et du schéma de rusanov, dans chaque code et à l'interface de couplage, conduit à une maximisation des effets de diffusion numérique, ce qui est favorable à la qualité des résultats.

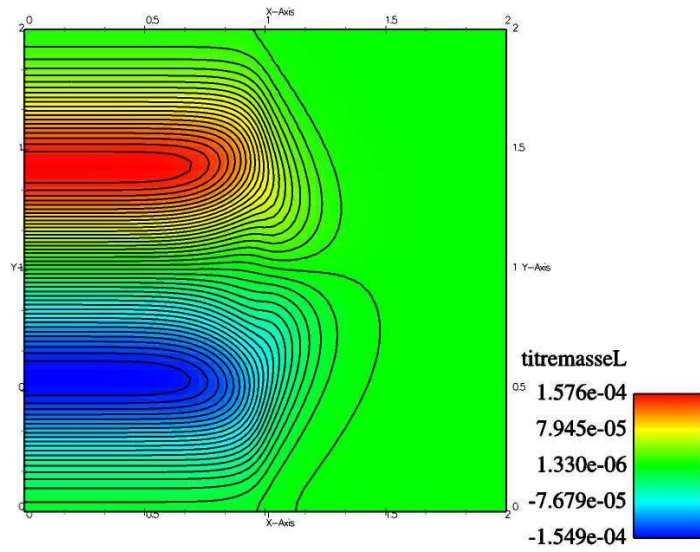


FIG. 5.2 – Isovaleurs du pourcentage de l'écart relatif du titre masse par rapport à 0.999518.

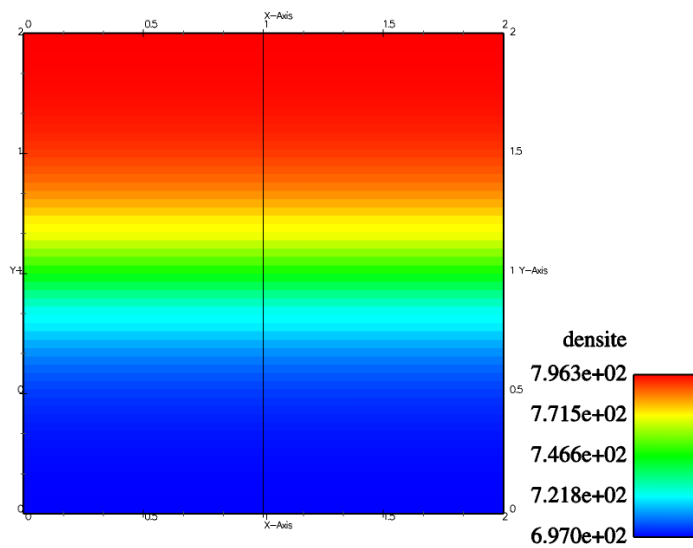


FIG. 5.3 – Isovaleurs de la densité du mélange $\rho = \alpha_l \rho_l + \alpha_v \rho_v$.

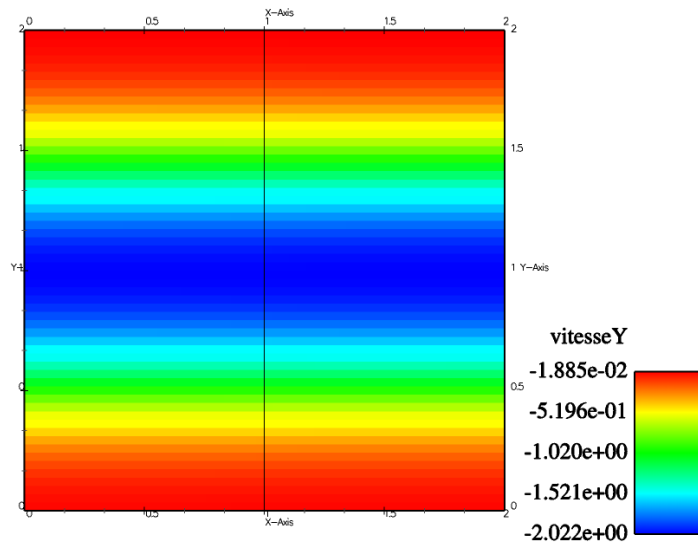


FIG. 5.4 – Isovaleurs de la composante de vitesse V_y du mélange $(\alpha_l \rho_l U_l + \alpha_v \rho_v U_v)/\rho$.

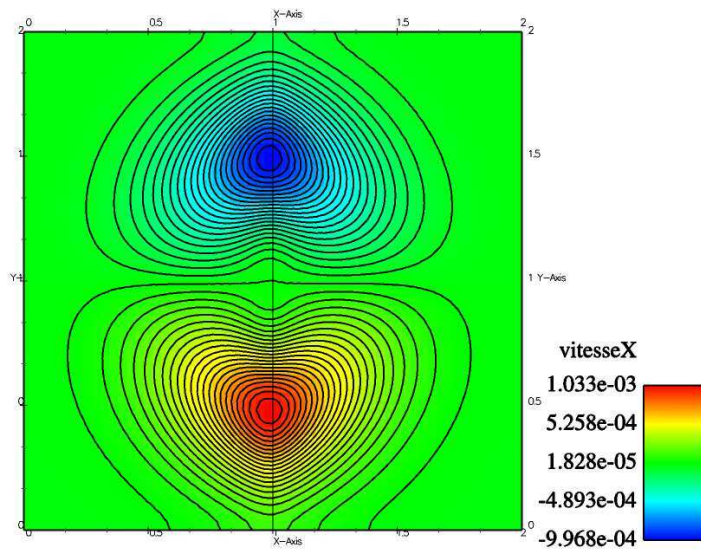


FIG. 5.5 – Isovaleurs de la composante de vitesse V_x du mélange $(\alpha_l \rho_l U_l + \alpha_v \rho_v U_v)/\rho$.

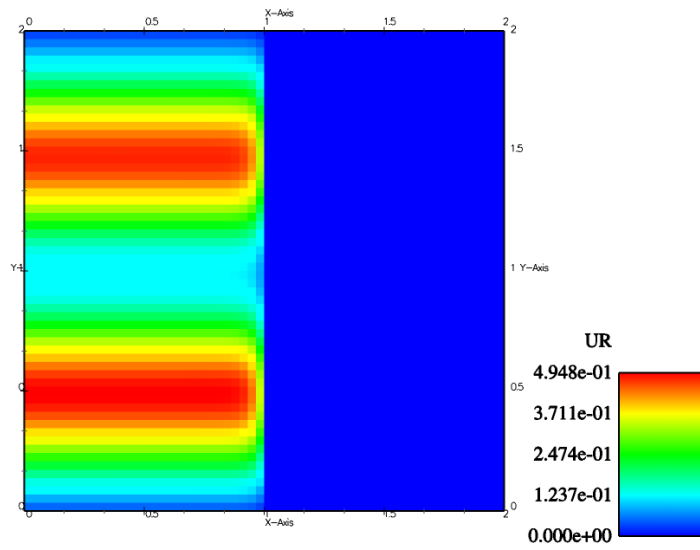


FIG. 5.6 – Isovaleurs de la composante de vitesse relative UR_y du mélange $U_v - U_l$

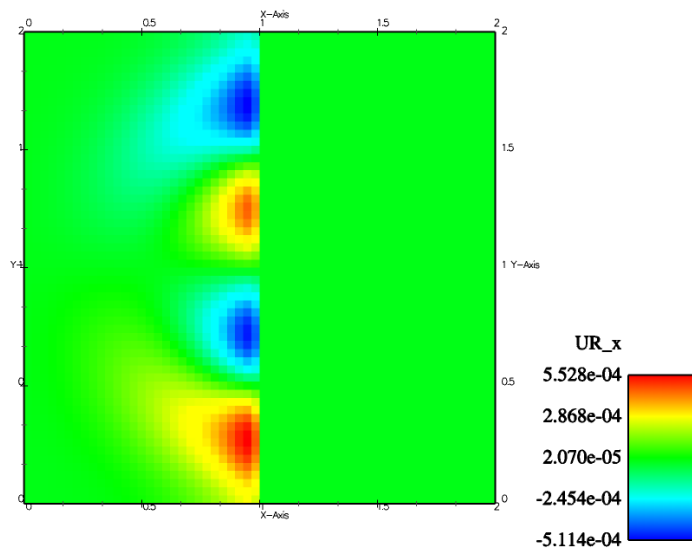


FIG. 5.7 – Isovaleurs de la composante de vitesse relative UR_x du mélange $U_v - U_l$

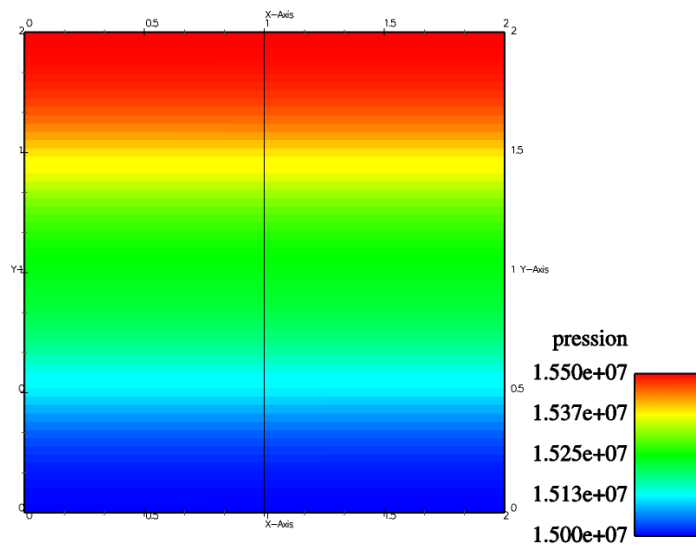


FIG. 5.8 – Isovaleurs de la pression P du mélange

Remarque. *Le même cas test a été réalisé en couplant le code HRM avec le code NEPTUNE_CFD. Le schéma de discrétisation de NEPTUNE_CFD étant très distinct de celui du code HRM, les fronts d'ondes rapides sont approximés de manière différente, créant dès lors des gradients discrets normaux à l'interface assez importants (en pression notamment). Il en résulte des courants transverses à l'interface d'amplitude très nettement supérieure. Il faut remarquer que cette tendance est également observée si l'on considère deux schémas décentrés différents de part et d'autre de l'interface, ou un maillage de taille très distincte dans chaque code, le long de la surface d'interface.*

5.6.2 Cas tests mono-dimensionnels

Contrairement au cas test précédent et à l'instar des cas tests du chapitre 4, on s'intéresse ici à la propagation d'ondes impactant l'interface de couplage de façon orthogonale. L'objectif est d'examiner les ondes réfléchies et les ondes transmises ainsi que la pollution stationnaire localisée sur l'interface de couplage. Les paramètres des lois d'état sont identiques au cas précédent.

On débute par une série de quatre problèmes de Riemann générant des ondes déclenchées en $x = 0.15$ ou $x = -0.15$ qui iront impacter l'interface de couplage. Les conditions initiales et les paramètres thermodynamiques sont les mêmes que pour le cas test précédent. Le domaine de calcul est l'intervalle $x \in [-1,1]$. L'interface de couplage se situe à $x = 0$, l'intervalle $[-1,0[$ correspond au domaine de simulation du modèle six équations tandis que le modèle HRM est simulé dans l'intervalle $]0,1]$. Trois maillages uniformes ont été utilisés : un maillage de type industriel contenant 100 mailles, un maillage fin constitué de 10000 cellules et un maillage intermédiaire de 500 cellules. La durée physique du calcul est de 0.0025s.

Les second et quatrième cas tests correspondent à la traversée d'une onde de détente et de choc du domaine HRM vers le domaine du modèle six équations. Les premier et troisième cas tests constituent l'équivalent de ceux-ci lorsque les ondes sont générées dans le domaine bi-fluide.

Pour chaque cas test, les courbes pour le titre masse liquide, la vitesse moyenne, la pression et la densité moyenne ont été regroupées de deux manières différentes :

- les solutions calculées pour les codes HRM et bi-fluide standard sur l'ensemble du domaine $[-1,1]$ et la solution couplée sont regroupées pour un même maillage ((5.9), (5.10), (5.11));
- les solutions couplées sont tracées pour chacun des trois maillages sur le même graphique.

Seule la variable titre masse liquide permet de distinguer les calculs HRM pur, bi-fluide pur et le cas couplé. Une onde de très faible amplitude reste "accrochée" sur l'interface de couplage. Une animation du phénomène instationnaire permet de vérifier que cette onde qui reste bloquée dans le domaine de calcul bi-fluide tend à s'évanouir quand t croît.

CAS1:

	bi-fluide	bi-fluide	HRM
α_l	0.995	0.995	0.995
ρ_l	800	700	700
U_l	0	0	0
P_l	155e5	150e5	150e5
ρ_v	76.667	67.083	67.083
U_v	0	0	0
P_v	155e5	150e5	150e5

CAS2:

	bi-fluide	HRM	HRM
α_l	0.995	0.995	0.995
ρ_l	800	800	700
U_l	0	0	0
P_l	155e5	155e5	150e5
ρ_v	76.667	76.667	67.083
U_v	0	0	0
P_v	155e5	155e5	150e5

CAS3:

	bi-fluide	bi-fluide	HRM
α_l	0.995	0.995	0.995
ρ_l	700	800	800
U_l	0	0	0
P_l	150e5	155e5	155e5
ρ_v	67.083	76.667	76.667
U_v	0	0	0
P_v	150e5	155e5	155e5

CAS4:

	bi-fluide	HRM	HRM
α_l	0.995	0.995	0.995
ρ_l	700	700	800
U_l	0	0	0
P_l	150e5	150e5	155e5
ρ_v	67.083	67.083	76.667
U_v	0	0	0
P_v	150e5	150e5	155e5

Avec de telles conditions initiales, le titre masse liquide est discontinu. Cette discontinuité est le reflet de la discontinuité des densités : pour $\rho_l = 800$ le titre masse liquide est égal à 0.999518652481 et pour $\rho_l = 700$ le titre masse liquide est égal à 0.999518652661.

Quels que soient la nature de l'onde (au sens de la solution HRM) et le sens de propagation de l'onde qui impacte l'interface de couplage, les résultats obtenus sont très satisfaisants. La solution obtenue par couplage est très proche de la solution monomodèle correspondant dans chacun des domaines. Pour les variables densité moyenne, vitesse moyenne, vitesse relative et pression les différences entre les trois simulations restent infimes et les ondes réfléchies sont d'amplitude très faible.

En revanche, pour le titre masse, les solutions calculées selon les trois méthodes sont très différentes. A l'échelle des variations de la solution obtenue par le modèle bi-fluide, la solution fournie par le modèle HRM est stationnaire. La première présente deux bosses. L'extremum de la solution bi-fluide qui apparaît dans le domaine HRM reste localisé en $x = 0$ dans le cas de la solution couplée. Son amplitude est tout d'abord plus importante puis elle rejoint le niveau qu'elle aurait eu dans le cas d'un modèle bi-fluide.

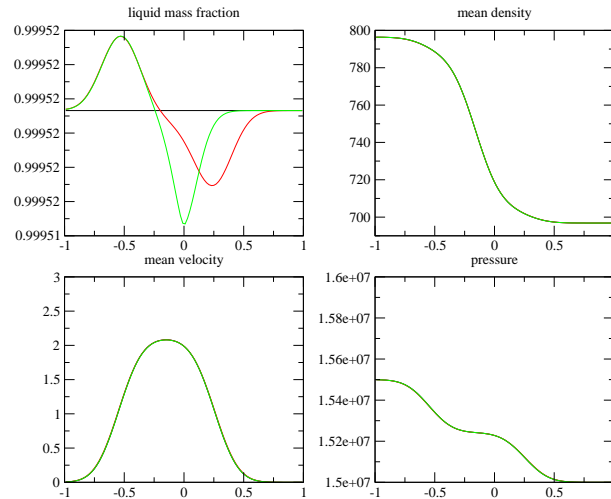


FIG. 5.9 – Premier cas test sur un maillage de 100 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

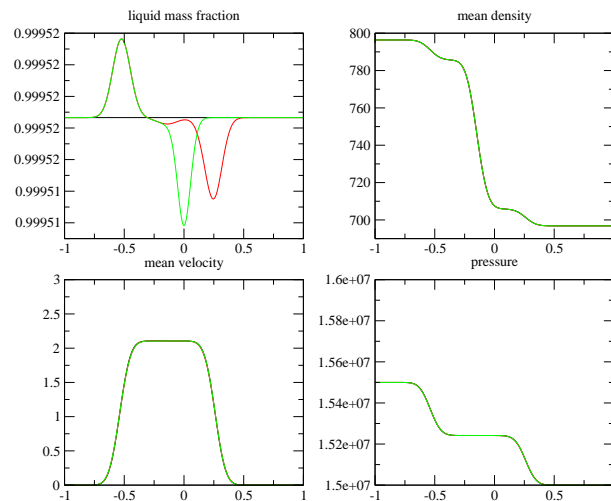


FIG. 5.10 – Premier cas test sur un maillage de 500 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

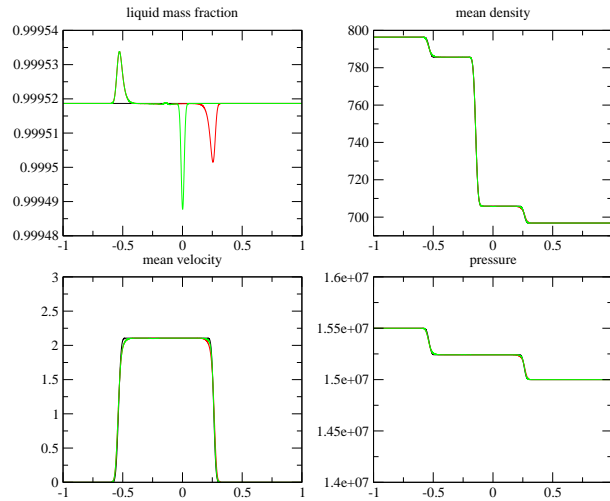


FIG. 5.11 – Premier cas test sur un maillage de 10000 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

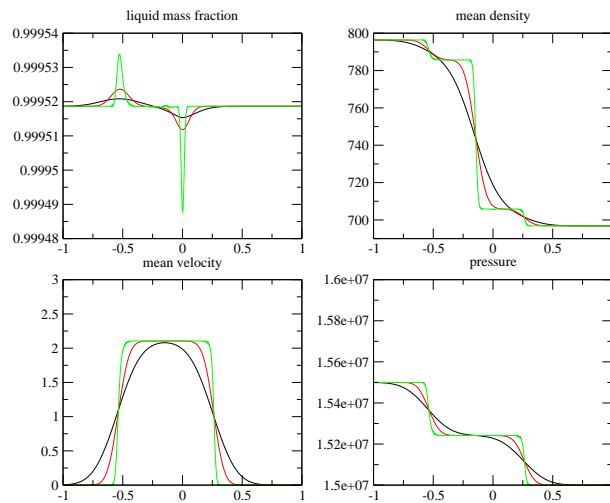


FIG. 5.12 – Premier cas test regroupant les cas couplés sur maillage à 100, 500 et 10000 mailles (noir, rouge, vert respectivement)

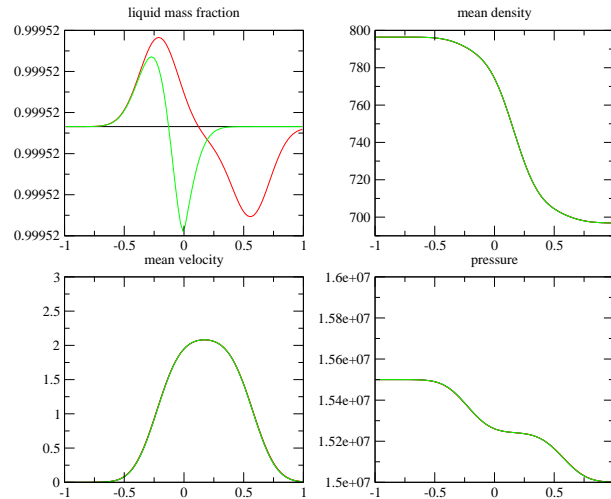


FIG. 5.13 – Deuxième cas test sur un maillage de 100 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

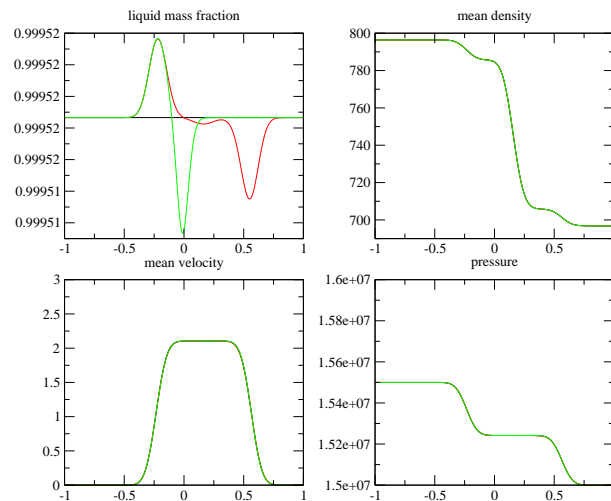


FIG. 5.14 – Deuxième cas test sur un maillage de 500 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

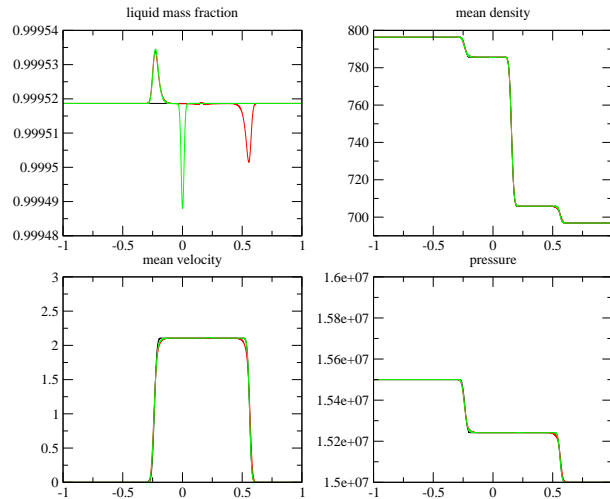


FIG. 5.15 – Deuxième cas test sur un maillage de 10000 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

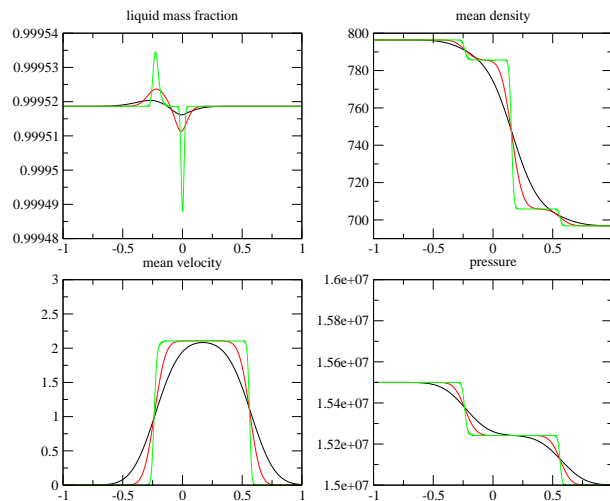


FIG. 5.16 – Deuxième cas test regroupant les cas couplés sur maillage à 100, 500 et 10000 mailles (noir, rouge, vert respectivement)

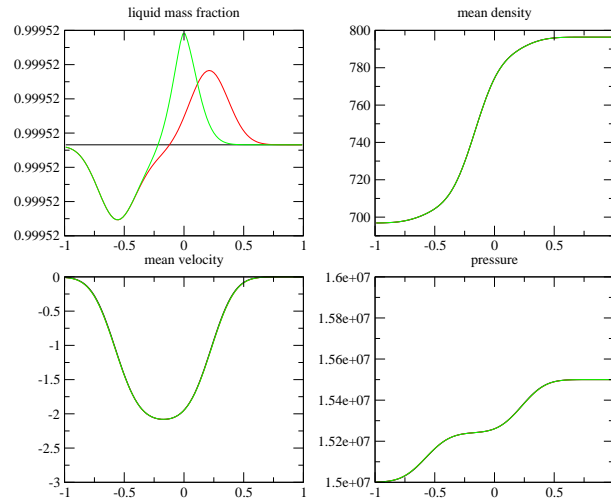


FIG. 5.17 – Troisième cas test sur un maillage de 100 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

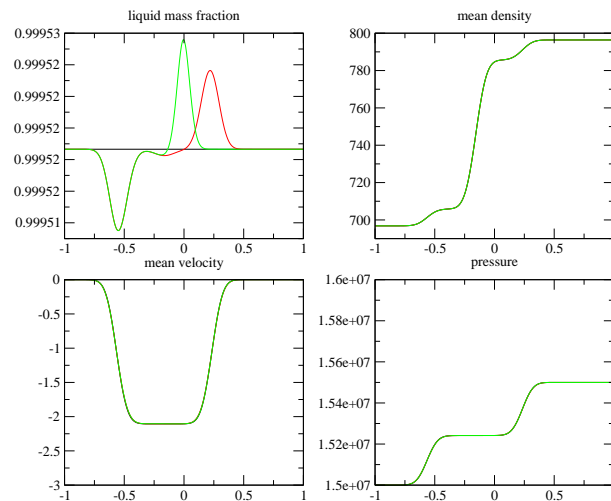


FIG. 5.18 – Troisième cas test sur un maillage de 500 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

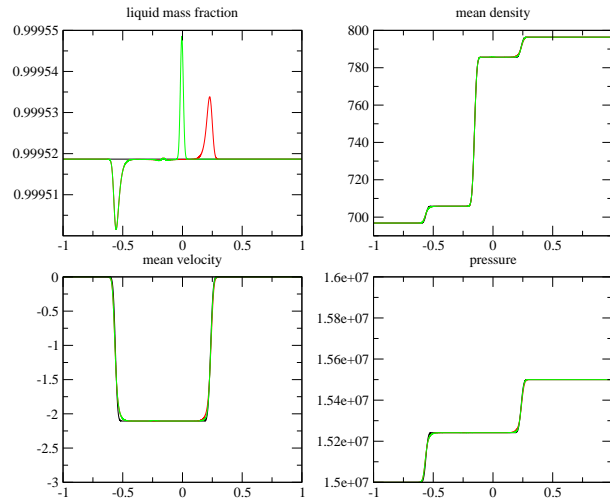


FIG. 5.19 – Troisième cas test sur un maillage de 10000 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

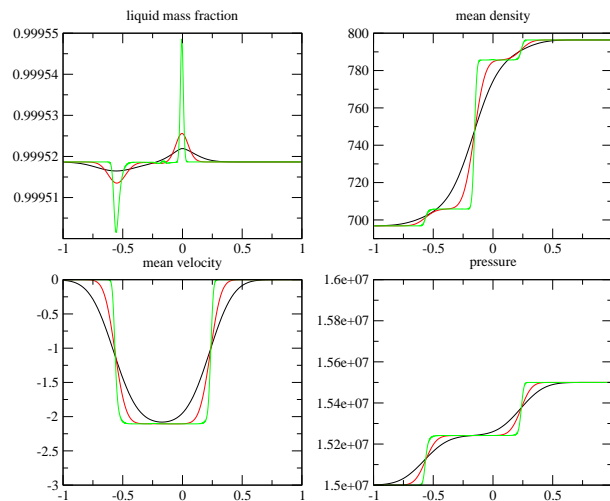


FIG. 5.20 – Troisième cas test regroupant les cas couplés sur maillage à 100, 500 et 10000 mailles (noir, rouge, vert respectivement)

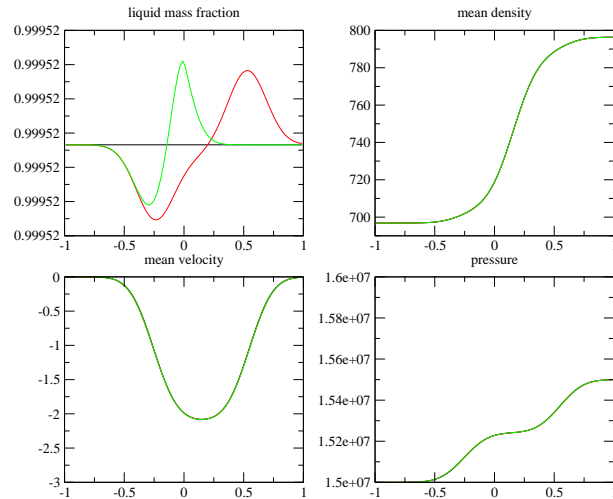


FIG. 5.21 – Quatrième cas test sur un maillage de 100 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

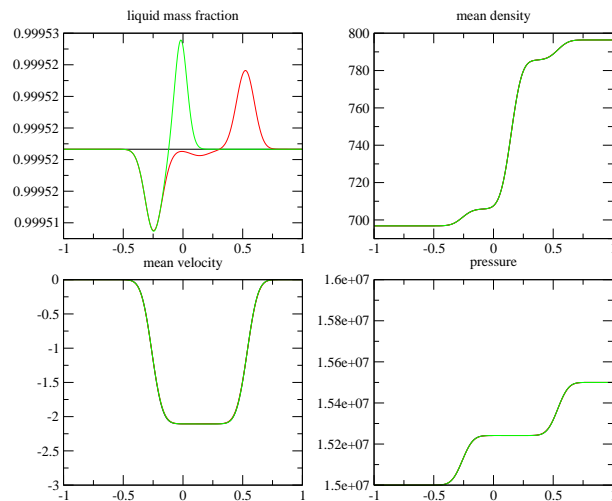


FIG. 5.22 – Quatrième cas test sur un maillage de 500 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

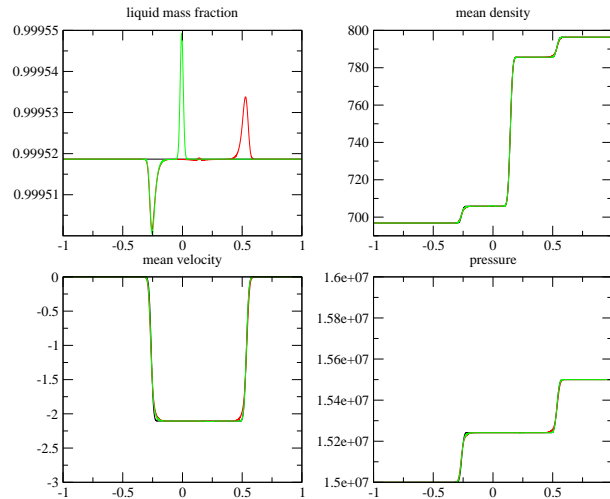


FIG. 5.23 – Quatrième cas test sur un maillage de 10000 mailles - noir=HRM, rouge=bi-fluide, vert=couplé

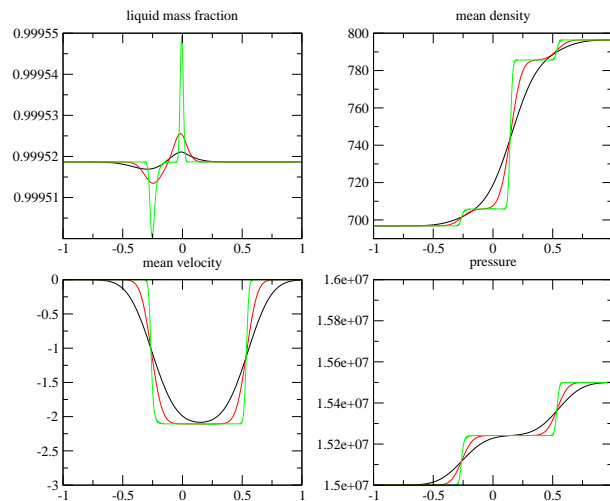


FIG. 5.24 – Quatrième cas test regroupant les cas couplés sur maillage à 100, 500 et 10000 mailles (noir, rouge, vert respectivement)

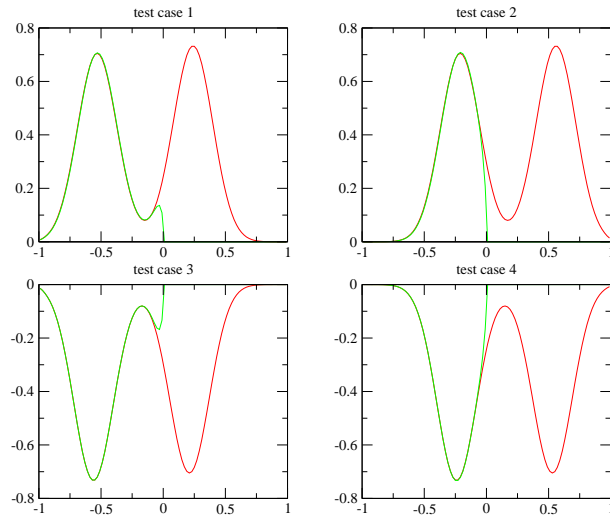


FIG. 5.25 – Vitesse relative sur maillage de 100 mailles pour les quatre cas tests - noir=HRM, rouge=bi-fluide, vert=couplé

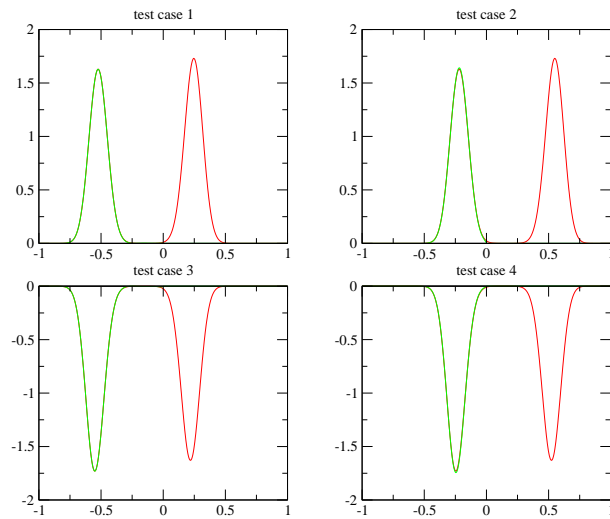


FIG. 5.26 – Vitesse relative sur maillage de 500 mailles pour les quatre cas tests - noir=HRM, rouge=bi-fluide, vert=couplé

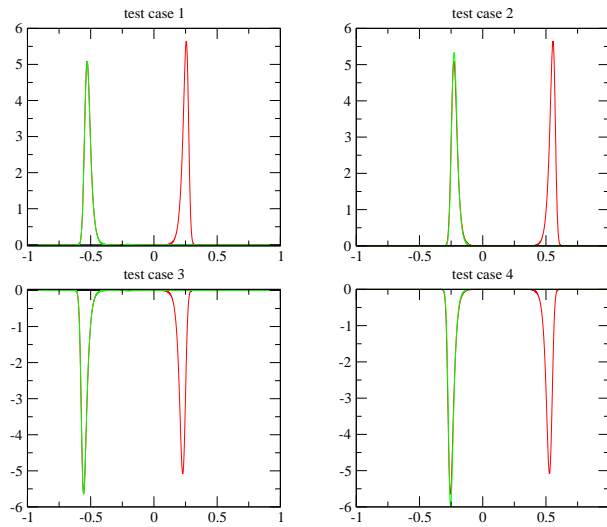


FIG. 5.27 – Vitesse relative sur maillage de 10000 mailles pour les quatre cas tests - noir=HRM, rouge=bi-fluide, vert=couplé

5.6.3 Effet de la traînée sur la qualité du couplage

Le maillage utilisé comporte 500 mailles uniformes. La CFL est toujours de 0.5. Les données initiales sont celles du premier cas test de la section précédente. Le paramètre τ_3 prend successivement les valeurs suivantes $\{10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}\}$.

On cherche ici à étudier l'influence du coefficient de traînée sur la qualité du calcul couplé. On attend *a priori* à retrouver une tendance à la régularisation lorsque l'échelle de temps diminue. Cet effet est effectivement retrouvé sur la base des résultats numériques présentés.

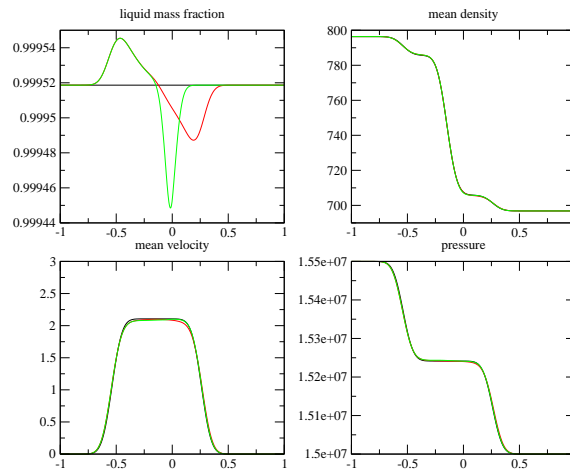


FIG. 5.28 – Premier cas test sur un maillage de 500 mailles avec $\tau_3 = 10^{-3}$ - noir=HRM, rouge=bi-fluide, vert=couplé

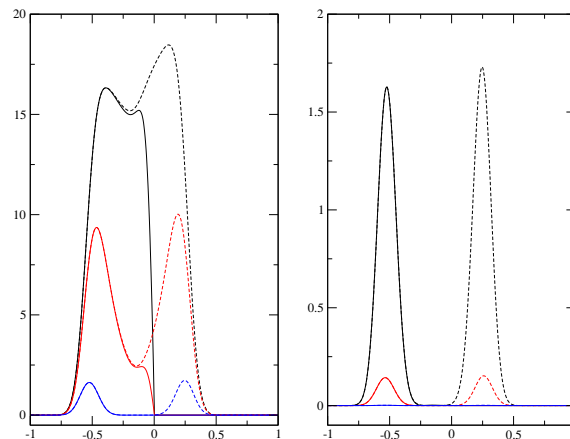


FIG. 5.29 – Vitesses relatives. La figure de gauche regroupe les résultats pour $\tau_3 = 10^{-2}$ en noir, pour $\tau_3 = 10^{-3}$ en rouge et pour $\tau_3 = 10^{-4}$ en bleu. La figure de droite regroupe les résultats pour $\tau_3 = 10^{-4}$ en noir, pour $\tau_3 = 10^{-5}$ en rouge et pour $\tau_3 = 10^{-6}$ en bleu. Pour les deux graphiques les lignes pointillées représentent les solutions obtenues pour le modèle bi-fluide standard sur l'ensemble du domaine et les lignes pleines correspondent aux solutions couplées.

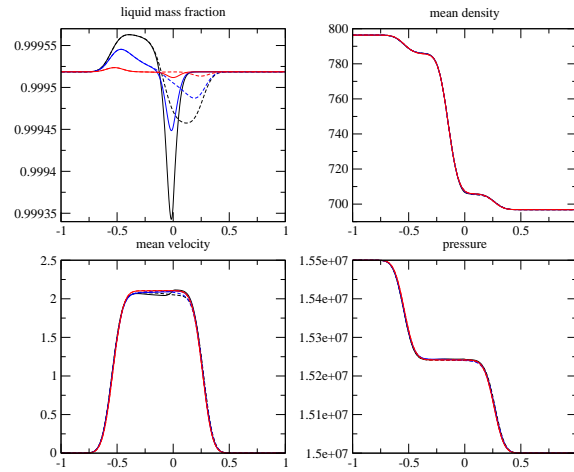


FIG. 5.30 – Cette figure regroupe les résultats pour $\tau_3 = 10^{-2}$ en noir, pour $\tau_3 = 10^{-3}$ en bleu et pour $\tau_3 = 10^{-4}$ en rouge. Les lignes pointillées représentent les solutions obtenues pour le modèle bi-fluide standard sur l'ensemble du domaine et les lignes pleines correspondent aux solutions couplées.

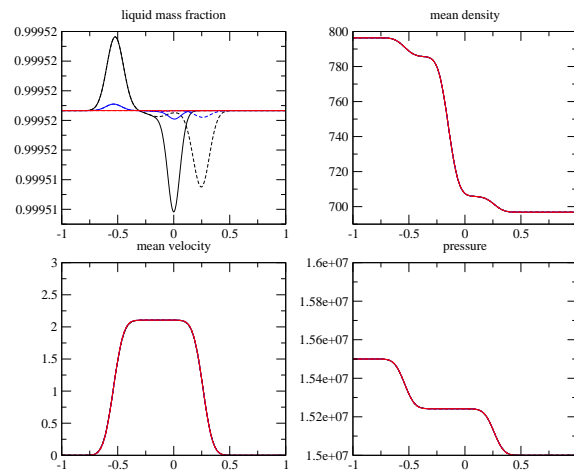


FIG. 5.31 – Cette figure regroupe les résultats pour $\tau_3 = 10^{-4}$ en noir, pour $\tau_3 = 10^{-5}$ en bleu et pour $\tau_3 = 10^{-6}$ en rouge. Les lignes pointillées représentent les solutions obtenues pour le modèle bi-fluide standard sur l'ensemble du domaine et les lignes pleines correspondent aux solutions couplées.

Remarque. *Formellement, lorsque les échelles τ_3 et τ_4 s'évanouissent, les modèles bi-fluide et HRM sont identiques. Pour des conditions initiales semblables, les approximations convergées seront a priori identiques. Ce résultat est effectivement retrouvé à convergence en maillage, tout au moins lorsque le transfert de masse est absent de la simulation.*

5.6.4 Cas test d'interaction entre une conduite et une cuve

On examine ici le cas d'une cuve bidimensionnelle où le modèle régissant les évolutions du fluide est le modèle HRM, tandis que le code correspondant à la conduite unidimensionnelle calcule des approximations des solutions du modèle bi-fluide. L'interface de couplage est situé au plus mauvais endroit (voir chapitre 3), soit au niveau du raccord géométrique entre la cuve et la conduite.

Le domaine de calcul est identique à celui utilisé au chapitre 3 (voir figure 3.4 par exemple) et contient 7140 mailles. La CFL est de 0.5. Les conditions initiales sont les suivantes:

$$\text{Si } (x-1)^2 + y^2 < 0.5 \text{ alors } \begin{cases} \alpha_l = 0.95 \\ \rho_l = 1000 \\ U_l = V_l = 0 \\ P_l = 160.10^5 \\ \rho_v = \rho_l \frac{(\gamma_l-1)C_{V,l}}{(\gamma_v-1)C_{V,v}} \\ U_v = V_v = 0 \\ P_v = 160.10^5 \end{cases} \quad \text{sinon } \begin{cases} \alpha_l = 0.95 \\ \rho_l = 900 \\ U_l = V_l = 0 \\ P_l = 150.10^5 \\ \rho_v = \rho_l \frac{(\gamma_l-1)C_{V,l}}{(\gamma_v-1)C_{V,v}} \\ U_v = V_v = 0 \\ P_v = 150.10^5 \end{cases} \quad (5.48)$$

où $\gamma_l = \gamma_v = 1.8$, $C_{V,l} = 3036$ et $C_{V,v} = 31680$.

Les animations seront accessibles sur le site :

http://www.cmi.univ-mrs.fr/~hurisse/simulation_numerique.html.

5.7 Prise en compte du transfert de masse

5.7.1 Un cas test mono-dimensionnel

Les paramètres des lois d'état sont toujours ceux des deux premières sections:

$$\gamma_l = \gamma_v = 1.24 \quad \text{et} \quad P_{\infty,l} = P_{\infty,v} = 0$$

$$C_{V,l} = 3036 \quad \text{et} \quad C_{V,v} = 31680$$

On néglige ici encore le transfert de chaleur sans transfert de masse, en posant $(\tau_4)^{-1} = 0$. On choisit le paramètre de relaxation en vitesse suivant : $\tau_3 = 10^{-4}$. On examine ici l'influence de la prise en compte du transfert de masse.

Sur un maillage de 500 mailles, on effectue la simulation du premier cas test mono-dimensionnel, en fixant $\tau_1 = 10^{-3}$. On trace à $T = 0.0025$ les résultats associés au cas bi-fluide seul, au modèle HRM seul et au cas couplé lorsque l'interface de couplage est située en $x = 0$. On note sur la figure (5.32) un effet de dérive entre le titre de masse asymptotique à droite dans le code HRM et à gauche dans le cadre bi-fluide. L'absence de terme de rappel en température, associé au déséquilibre cinématique dans le domaine bi-fluide est à l'origine de ce phénomène. La solution couplée s'efforce de régulariser le profil de titre masse associé. L'écart observé sur les bords du domaine entre le calcul couplé et son homologue mono-modèle est dû au décalage temporel de la simulation, et se résorbe en maillage. Il faut noter que la vitesse relative est toujours assez importante (de l'ordre de la vitesse moyenne).

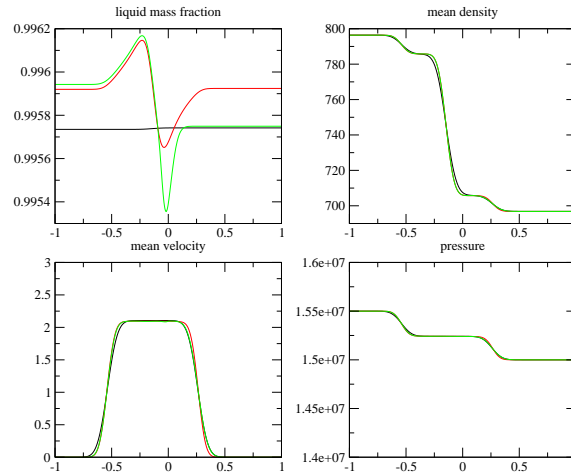


FIG. 5.32 – *Prise en compte du transfert de masse sur la base des conditions initiales du cas 1 - 500 mailles - noir=HRM, rouge=bi-fluide, vert=couplé*

En considérant toujours un maillage de 500 mailles, on réalise des simulations à condition initiale identique, mais lorsque τ_1 prend les valeurs suivantes: $\tau_1 = 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$. Deux blocs se distinguent. Le premier correspond aux deux échelles de temps les plus longues. Le titre masse liquide varie alors assez peu dans la simulation, présentée pour un temps final $T = 0.0025$. Inversement, les deux valeurs les plus faibles conduisent à une chute du titre masse très importante, dans les zones de plus faible pression (voir figure (5.33)). Sur cette configuration typiquement, l'utilisation

d'un schéma de Rusanov permet d'assurer la positivité de la masse partielle par maille. On note néanmoins que les bords de la zone de vide liquide sont assez mal représentés. D'autre part, l'interface de couplage est clairement identifiable sur la représentation en vitesse moyenne, en densité et en pression.

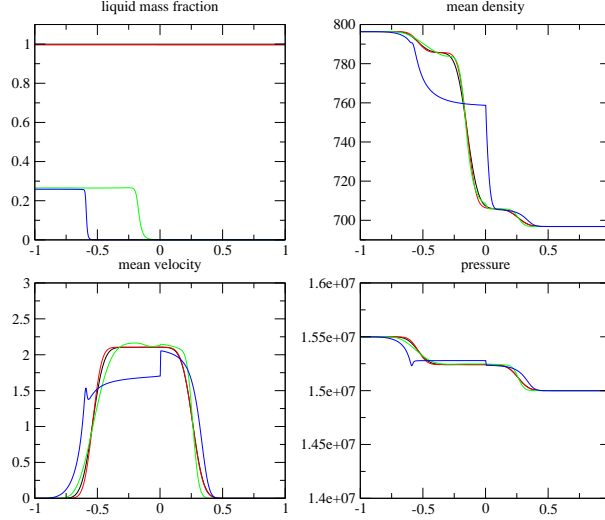


FIG. 5.33 – Prise en compte du transfert de masse sur la base des conditions initiales du cas 1 - 500 mailles - noir= 10^{-2} , rouge= 10^{-3} , vert= 10^{-4} , bleu= 10^{-5}

5.7.2 Cas test d'interaction entre une conduite et une cuve

On réalise un cas test similaire au cas test de la section 5.D, en effectuant un calcul couplant un domaine unidimensionnel et une cuve bidimensionnelle, ces deux domaines étant régis respectivement par le modèle bi-fluide et le modèle HRM. L'interface de couplage est située au niveau du raccord géométrique entre la cuve et le tuyau. Les conditions initiales correspondent à un déclenchement de problème de Riemann axisymétrique dans la cuve. On prend ici encore en compte le terme de transfert de masse, en choisissant la valeur : $\tau_1 = 10^{-2}$. L'échelle de temps de relaxation en vitesse est : $\tau_3 = 10^{-4}$. Les conditions initiales sont :

$$\text{Si } (x-1)^2 + y^2 < \frac{1}{3} \text{ alors } \begin{cases} \alpha_l = 0.95 \\ \rho_l = 800 \\ U_l = V_l = 0 \\ P_l = 155.10^5 \\ \rho_v = 76.667 \\ U_v = V_v = 0 \\ P_v = 155.10^5 \end{cases} \quad \text{sinon } \begin{cases} \alpha_l = 0.95 \\ \rho_l = 700 \\ U_l = V_l = 0 \\ P_l = 150.10^5 \\ \rho_v = 67.083 \\ U_v = V_v = 0 \\ P_v = 150.10^5 \end{cases} \quad (5.49)$$

Les paramètres thermodynamiques sont $\gamma_l = \gamma_v = 1.24$, $C_{V,l} = 3036$ et $C_{V,v} = 31680$. Le transfert de chaleur pur est toujours négligé, c'est-à-dire que l'on a $(\tau_4)^{-1} = 0$.

Les animations seront accessibles sur le site :

http://www.cmi.univ-mrs.fr/~hurisse/simulation_numerique.html.

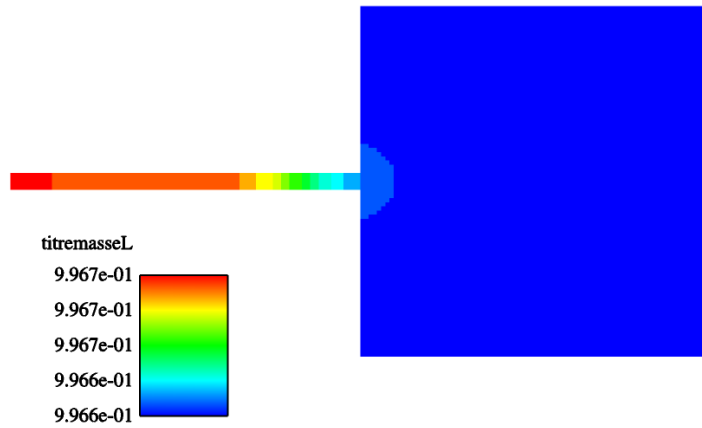


FIG. 5.34 – Isovaleurs du titre masse liquide, $\frac{\alpha_l \rho_l}{\alpha_l \rho_l + \alpha_v \rho_v}$

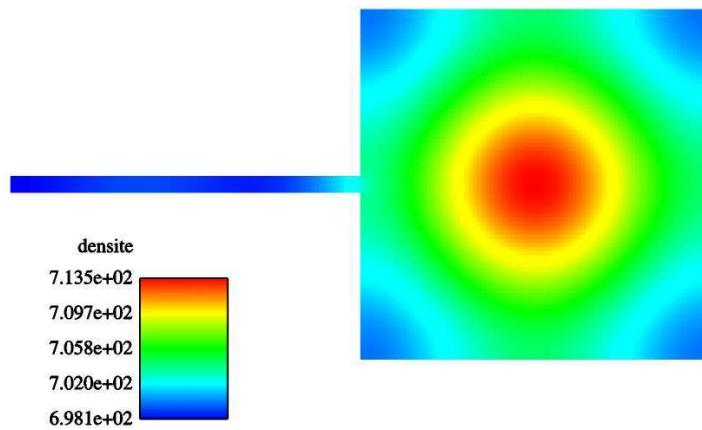


FIG. 5.35 – Isovaleurs de la densité moyenne, $\alpha_l \rho_l + \alpha_v \rho_v$

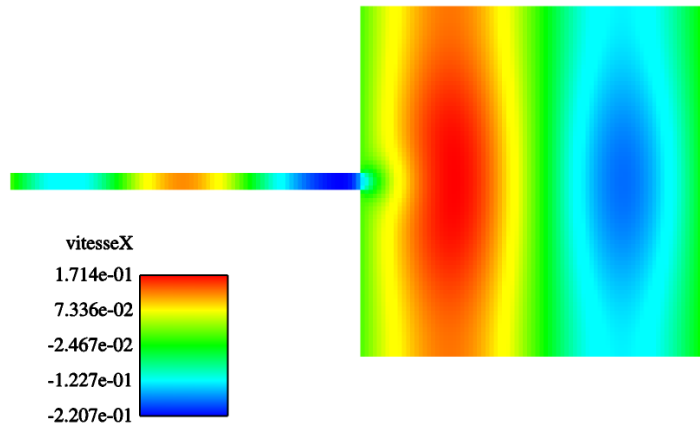


FIG. 5.36 – Isovaleurs de la composante horizontale de la vitesse de mélange, $\frac{\alpha_l \rho_l U_l + \alpha_v \rho_v U_v}{\alpha_l \rho_l + \alpha_v \rho_v}$

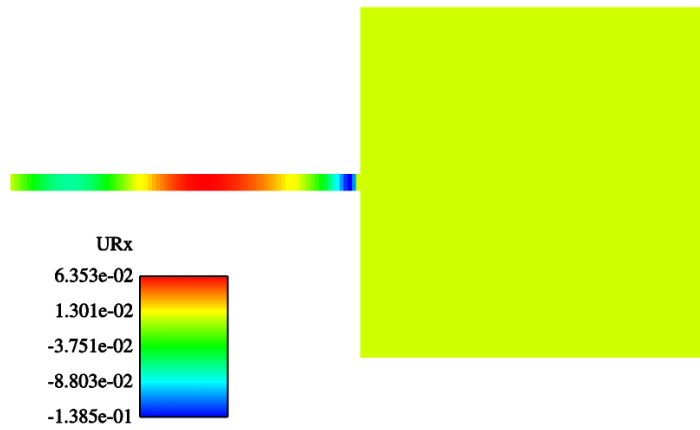


FIG. 5.37 – Isovaleurs de la composante horizontale de la vitesse relative, $U_l - U_v$

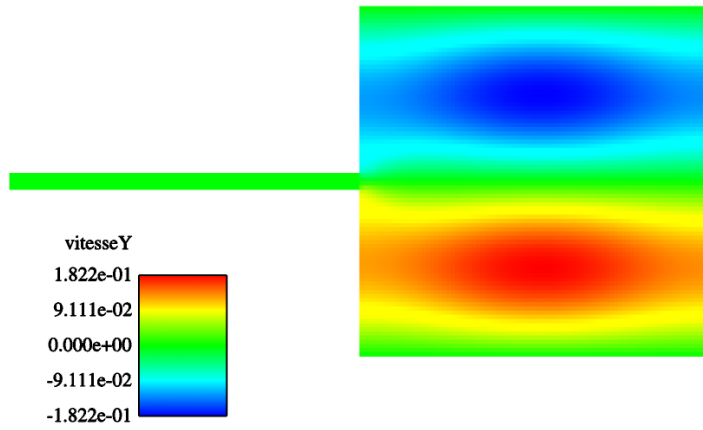


FIG. 5.38 – Isovaleurs de la composante verticale de la vitesse de mélange, $\frac{\alpha_l \rho_l U_l + \alpha_v \rho_v U_v}{\alpha_l \rho_l + \alpha_v \rho_v}$

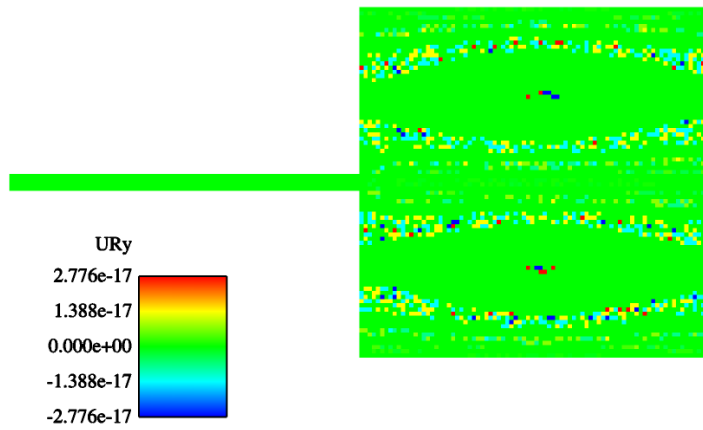


FIG. 5.39 – Isovaleurs de la composante verticale de la vitesse relative, $U_l - U_v$

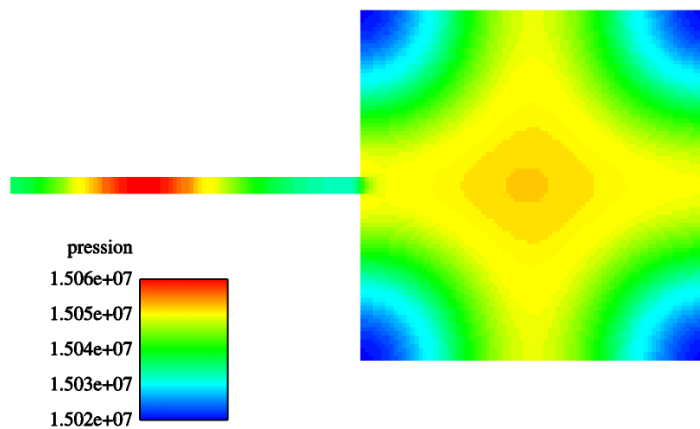


FIG. 5.40 – *Isovaleurs de la pression*

5.8 Conclusion

Sur l'ensemble des cas test réalisés (aucun d'entre eux ne faisant intervenir le transfert de chaleur pur, i.e. $(\tau_4)^{-1} = 0$), les solutions couplées obtenues sont semblables aux solutions obtenues pour le modèle HRM dans le domaine HRM et sont semblables aux solutions obtenues pour le modèle bi-fluide dans le domaine correspondant. De plus dans toutes les situations testées, l'algorithme proposé a fourni une solution satisfaisante.

Même si le terme de transfert de masse est identique pour les deux modèles, et compatible avec la thermodynamique, son introduction n'est pas sans conséquence. En effet pour les cas tests envisagés en l'absence de transfert de masse, la solution obtenue en simulant le modèle bi-fluide tend vers la solution calculée pour le modèle HRM lorsque la constante de temps du terme source de traînée tend vers zéro. Cette compatibilité n'est plus valable quand le transfert de masse est activé (voir section 6). De fait les solutions sont structurellement différentes (équilibres en vitesse et température pour le modèle HRM, ce qui n'est pas le cas pour le modèle bi-fluide), ce qui explique la dérive entre elles, qui est surtout visible sur le titre masse liquide. Hormis cette différence de comportement entre les deux modèles simulés, la solution couplée reste stable, même si l'interface de couplage devient "visible" lorsque l'échelle de temps de relaxation associée au transfert de masse devient faible.

La méthode de simulation présentée dans ce chapitre, qui est basée sur des techniques de relaxation d'un modèle père, semble être un outil très puissant. En ce qui concerne les perspectives, on pourrait envisager de simuler tout un ensemble de modèles fils en utilisant un modèle père suffisamment général, et même de les coupler entre eux. Les algorithmes associés étant très modulaires, ils sont facilement modifiables, et le code de calcul associé peut facilement rester général.

Ce travail est un travail préliminaire et les méthodes qui y sont exposées méritent une étude nettement plus complète. Les connaissances actuelles sur le modèle bi-fluide standard, sur le modèle bi-fluide à deux pressions et sur la méthode de simulation par relaxation d'un modèle à partir d'un modèle père restent à approfondir.

5.9 Appendix 1 : Le schéma VFRoe-ncv en variable

$$Q = (Y, \alpha_l, s_l, U_l, P_l, s_v, U_v, P_v)^\top$$

La méthode de couplage décrite dans le corps du chapitre nécessite de calculer une valeur d'interface pour les grandeurs physiques. Ceci est réalisé grâce à un schéma VFRoe-ncv [16] utilisant le jeu de variables $Q = (Y, \alpha_l, s_l, U_l, P_l, s_v, U_v, P_v)^\top$ appliqué à la partie convective du système d'équations (5.41) du modèle d'interface.

On rappelle que les lois de fermetures sont telles que l'on a :

$$V_I = U_v \quad \text{et} \quad P_I = P_l$$

En considérant le jeu de variables Q , la matrice de convection $J(Q)$ du système (5.41) est :

$$J(Q) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & U_v & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & U_l & 0 & 0 & 0 & 0 & 0 \\ 0 & q_l & 0 & U_l & 1/\rho_l & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{\gamma}_l P_l & U_l & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & U_v & 0 & 0 \\ 0 & q_v & 0 & 0 & 0 & 0 & U_v & 1/\rho_v \\ 0 & 0 & 0 & 0 & 0 & 0 & \hat{\gamma}_v P_v & U_v \end{pmatrix}$$

où les termes q_l et q_v permettent de coupler les deux sous-systèmes d'équations liquide et vapeur :

$$q_l = \frac{\hat{\gamma}_l P_l}{\alpha_l} (U_l - U_v)$$

$$q_v = \frac{(P_l - P_v)}{\alpha_v \rho_v}$$

On pose de plus :

$$b = \frac{q_l}{\rho_l (c_l^2 - (U_l - U_v)^2)}$$

Remarque. Les termes q_l , q_v , b , $\hat{\gamma}_l$ ainsi que les densités phasiques doivent se lire comme des fonctions de Q , pour ne pas rendre les formules illisibles, l'argument sera omis. Les densités phasiques s'expriment en fonction de Q , dans le cadre de deux lois d'état de type gaz raides on a pour $\phi = l, v$:

$$\rho_\phi(Q) = \left[(P_\phi + P_{\infty, \phi}) e^{(-s_\phi / C_{V, \phi})} - C_{V, \phi} \right]$$

et la célérité du son est défini par :

$$\rho_\phi(Q) c_\phi(Q)^2 = \hat{\gamma}_\phi(Q) P_\phi = \gamma_\phi (P_\phi + P_{\infty, \phi})$$

Les valeurs propres et les vecteurs propres de la matrice de convection J sont :

$$\begin{aligned}
 \lambda_0 &= 0; & r_0^\top &= (1,0,0,0,0,0,0,0) \\
 \lambda_1 &= U_v; & r_1^\top &= (0,1,0, -b, \rho_l(U_l - U_v)b, 0, 0, -\rho_v q_v) \\
 \lambda_2 &= U_l - c_l; & r_2^\top &= (0,0,0,1, -\rho_l c_l, 0, 0, 0) \\
 \lambda_3 &= U_v; & r_3^\top &= (0,0,1,0,0,0,0,0) \\
 \lambda_4 &= U_l + c_l; & r_4^\top &= (0,0,0,1, \rho_l c_l, 0, 0, 0) \\
 \lambda_5 &= U_l - c_l; & r_5^\top &= (0,0,0,0,0,0,1, -\rho_v c_v) \\
 \lambda_6 &= U_v; & r_6^\top &= (0,0,0,0,0,1,0,0) \\
 \lambda_7 &= U_l + c_l; & r_7^\top &= (0,0,0,0,0,1, \rho_v c_v)
 \end{aligned}$$

Soit Ω la matrice dont les colonnes sont les vecteurs propres r_k pour $k = 0..7$, autrement dit la matrice de passage de la base canonique vers la base des vecteurs propres, $\Omega(Q) = (r_0; r_1; r_3; r_2; r_4; r_6; r_5; r_7)$ (les indices sont volontairement desordonnés).

Le schéma VFRoe-ncv est basé sur la résolution du problème de Riemann linéarisé associé à la matrice $J(\bar{Q})$ et aux états droit Q_R et gauche Q_L . L'état \bar{Q} est un état moyen que l'on choisit classiquement comme la moyenne arithmétique des états droit et gauche (d'autres choix sont possibles), c'est-à-dire,

$$\bar{Q} = \frac{Q_R + Q_L}{2}$$

On cherche à définir la solution en $x/t = 0$ du problème de Riemann :

$$\partial_t(Q) + J(\bar{Q})\partial_x(Q) = 0, \quad \text{avec} \quad Q(x, t = 0) = \begin{cases} Q_L & \text{si } x < 0 \\ Q_R & \text{si } x > 0 \end{cases} \quad (5.50)$$

On définit le vecteur $\zeta = (\zeta_0, \zeta_1, \zeta_3, \zeta_2, \zeta_4, \zeta_6, \zeta_5, \zeta_7)^\top$ par la formule :

$$\zeta = \Omega^{-1}(\bar{Q})(Q_R - Q_L)$$

où Ω^{-1} est l'inverse de la matrice Ω et s'exprime de la façon suivante :

$$\Omega^{-1}(Q) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{b(c_l + U_l - U_v)}{2c_l} & 0 & \frac{-1}{2} & \frac{-1}{2\rho_l c_l} & 0 & 0 & 0 \\ 0 & \frac{b(c_l - U_l + U_v)}{2c_l} & 0 & \frac{1}{2} & \frac{1}{2\rho_l c_l} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & \frac{-q_v}{2c_v} & 0 & 0 & 0 & 0 & \frac{-1}{2} & \frac{-1}{2\rho_v c_v} \\ 0 & \frac{q_v}{2c_v} & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2\rho_v c_v} \end{pmatrix}$$

Dans la classe des fonctions auto-similaires, la solution de (5.50) est :

$$Q(x/t) = Q_L + \sum_{\lambda_k < x/t} \zeta_k r_k(\bar{Q}) = Q_R - \sum_{\lambda_k > x/t} \zeta_k r_k(\bar{Q}) \quad (5.51)$$

5.10 Appendix 2: Intégration numérique des termes sources physiques pour le modèle bifluide à deux pressions

Dans le cadre des méthodes de relaxation présentées ci-dessus, les termes sources physiques du modèle bifluide à deux pressions sont de nature différente. Il y a :

- le transfert de masse associé à Γ ;
- le terme d'équilibrage des vitesses phasiques associé à \mathcal{B} ;
- le terme d'équilibrage des températures phasiques associé à \mathcal{C} .

Le terme \mathcal{A} est considéré comme un terme de relaxation instantanée dans les techniques permettant d'aboutir aux modèles à quatre et six équations. Chacun de ces trois effets est traité séparément. On présente dans ce qui suit une manière de mettre à jour les variables du système à sept équations pour chacun des effets ci-dessus pris *indépendamment*. On suppose que l'état initial de chacune des étapes est noté pour $t = t^n$:

$$(W^n)^\top = (\alpha_l, \alpha_l \rho_l, \alpha_l \rho_l U_l, \alpha_l E_l, \alpha_v \rho_v, \alpha_v \rho_v U_v, \alpha_v E_v)^n$$

on cherche à déterminer l'état à $t = t^n + \Delta t$

$$(W^{n+1})^\top = (\alpha_l, \alpha_l \rho_l, \alpha_l \rho_l U_l, \alpha_l E_l, \alpha_v \rho_v, \alpha_v \rho_v U_v, \alpha_v E_v)^{n+1}$$

On utilisera par ailleurs les notations suivantes pour les masses partielles :

$$m_l = \alpha_l \rho_l \quad \text{et} \quad m_v = \alpha_v \rho_v$$

On suppose que m_l^n , m_v^n , $(m_l e_l)^n$ et $(m_v e_v)^n$ sont positives et que le titre liquide α^n est compris entre 0 et 1.

5.10.1 Le transfert de masse

On s'intéresse tout d'abord au transfert de masse qui est gouverné par le terme source Γ . Le système à résoudre est le suivant :

$$\begin{cases} \partial_t (\alpha_l) = 0 \\ \partial_t (m_l) = \Gamma \\ \partial_t (m_l U_l) = \Gamma V_I \\ \partial_t (\alpha_l E_l) = \Gamma H_I \\ \partial_t (m_v) = -\Gamma \\ \partial_t (m_v U_v) = -\Gamma V_I \\ \partial_t (\alpha_v E_v) = -\Gamma H_I \end{cases} \quad (5.52)$$

avec $H_I = V_I^2/2$, $V_I = U_v$ et :

$$\Gamma = (\tau_1)^{-1} \frac{1}{T_l^{-1} \mu_l + T_v^{-1} \mu_v} \frac{m_l m_v}{m_l + m_v} (T_l^{-1} \mu_l - T_v^{-1} \mu_v)$$

On fait le choix d'explicitier une partie de Γ . Celui-ci est donc remplacé par le terme :

$$J_l = (\theta_1^n)^{-1} \frac{m_l m_v}{m_l + m_v}$$

où l'on connaît de façon explicite le terme θ_1^n en fonction de W^n par la formule :

$$(\theta_1^n)^{-1} = (\tau_1)^{-1} \left[\frac{T_l^{-1}\mu_l - T_v^{-1}\mu_v}{T_l^{-1}\mu_l + T_v^{-1}\mu_v} \right]^n$$

Il reste alors à intégrer de manière exacte le système suivant :

$$\begin{cases} \partial_t (\alpha_l) = 0 \\ \partial_t (m_l) = J_l \\ \partial_t (m_l U_l) = J_l U_v \\ \partial_t (\alpha_l E_l) = J_l U_v^2 / 2 \\ \partial_t (m_v) = -J_l \\ \partial_t (m_v U_v) = -J_l U_v \\ \partial_t (\alpha_v E_v) = -J_l U_v^2 / 2 \end{cases} \quad (5.53)$$

La première équation du système (5.53) fournit la solution triviale :

$$\alpha_l(t) = \alpha_l(0) \quad (5.54)$$

Les deux équations sur les masses partielles forment un sous-système fermé dont la solution exacte est :

$$m_l(t) = m_l(0) \frac{m_l(0) + m_v(0)}{m_l(0) + m_v(0)e^{(-t/\theta_1^n)}} \quad (5.55)$$

$$m_v(t) = m_v(0) \frac{m_l(0) + m_v(0)}{m_l(0)e^{(t/\theta_1^n)} + m_v(0)} \quad (5.56)$$

On vérifie que la masse totale est conservée :

$$m_l(t) + m_v(t) = m_l(0) + m_v(0)$$

Les équations sur les quantités de mouvement fournissent les équations sur les vitesses phasiques :

$$\begin{cases} \partial_t (U_l) = \frac{J_l}{m_l} (U_v - U_l) \\ \partial_t (U_v) = 0 \end{cases} \quad (5.57)$$

En utilisant les solutions trouvées pour les masses partielles (5.55) et (5.56), on obtient les solutions pour les vitesses phasiques :

$$U_l(t) = U_v(0) + (U_l(0) - U_v(0)) \frac{m_l(0) + m_v(0)e^{(-t/\theta_1^n)}}{m_l(0) + m_v(0)} \quad (5.58)$$

$$U_v(t) = U_v(0) \quad (5.59)$$

La quantité de mouvement totale est conservée, on a en effet :

$$(m_l U_l + m_v U_v)(t) = (m_l U_l + m_v U_v)(0)$$

Les deux équations sur les énergies totales phasiques fournissent les équations suivantes portant sur les énergies internes phasiques :

$$\begin{cases} \partial_t (m_l e_l) = \frac{J_l}{2} (U_v - U_l)^2 \\ \partial_t (m_v e_v) = 0 \end{cases} \quad (5.60)$$

Les solutions de ces équations sont :

$$(m_l e_l)(t) = (m_l e_l)(0) + \frac{m_v(0)m_l(0)}{m_l(0) + m_v(0)} \frac{(U_l(0) - U_v(0))^2}{2} (1 - e^{(-t/\theta_1^n)}) \quad (5.61)$$

$$(m_v e_v)(t) = (m_v e_v)(0) \quad (5.62)$$

Ces solutions permettent de conserver l'énergie totale de l'ensemble du système :

$$(m_l e_l + m_l \frac{U_l^2}{2})(t) + (m_v e_v + m_v \frac{U_v^2}{2})(t) = (m_l e_l + m_l \frac{U_l^2}{2})(0) + (m_v e_v + m_v \frac{U_v^2}{2})(0)$$

La mise à jour de la variable W est réalisée en utilisant les solutions (5.54), (5.55), (5.56), (5.58), (5.59), (5.61) et (5.62) au temps $t = \Delta t$ et en prenant comme condition initiale ($t = 0$) les valeurs de W^n .

Remarque. On suppose que m_l^n , m_v^n , $(m_l e_l)^n$ et $(m_v e_v)^n$ sont positives et que le titre liquide α^n est compris entre 0 et 1. Dès lors:

- Le titre liquide α^{n+1} est compris entre 0 et 1.
- Grâce à la forme des formules (5.55) et (5.56), les masses partielles m_l^{n+1} et m_v^{n+1} sont positives.
- L'énergie interne vapeur $(m_v e_v)^{n+1}$ est positive.
- L'énergie interne liquide $(m_l e_l)^{n+1}$ n'est en revanche que conditionnellement positive. Si $\theta_1^n < 0$, le pas de temps doit respecter la condition :

$$\Delta t < |\theta_1^n| \ln \left(1 + \frac{2e_l^n (m_v^n + m_l^n)}{m_v^n (U_l^n - U_v^n)^2} \right)$$

Cette contrainte sur le pas de temps existe indépendamment du schéma, dans la mesure où la positivité de l'énergie interne de la phase vapeur n'est pas structurellement assurée par le modèle de transfert de masse.

Remarque. La méthode proposée ci-dessus de prise en compte du terme de transfert de masse est valable pour n'importe quelle loi d'état.

5.10.2 Intégration numérique des termes de trainée statique

Le terme de trainée est noté \mathcal{B} et s'exprime de la façon suivante :

$$\mathcal{B} = (\tau_3)^{-1} \frac{m_l m_v}{m_l + m_v} (U_v - U_l)$$

La prise en compte de ce terme se fait donc grâce au système :

$$\left\{ \begin{array}{l} \partial_t (\alpha_l) = 0 \\ \partial_t (m_l) = 0 \\ \partial_t (m_l U_l) = \mathcal{B} \\ \partial_t (\alpha_l E_l) = \mathcal{B} V_I \\ \partial_t (m_v) = 0 \\ \partial_t (m_v U_v) = -\mathcal{B} \\ \partial_t (\alpha_v E_v) = -\mathcal{B} V_I \end{array} \right. \quad (5.63)$$

Les première, deuxième et cinquième équations du système (5.63) fournissent les solutions pour le titre liquide et les masses partielles :

$$\alpha_l(t) = \alpha_l(0) \quad (5.64)$$

$$m_l(t) = m_l(0) \quad (5.65)$$

$$m_v(t) = m_v(0) \quad (5.66)$$

La conservation de la masse est assurée, de même que la positivité des titres et des masses partielles. Le terme source \mathcal{B} s'écrit alors :

$$\mathcal{B} = (\tau_3)^{-1} \frac{m_l(0) m_v(0)}{m_l(0) + m_v(0)} (U_v - U_l)(t)$$

Les deux équations portant sur les quantités de mouvement donnent un système fermé de deux équations au dérivées ordinaires linéaires portant sur les vitesses phasiques dont la solution est :

$$U_l(t) = \frac{m_l(0) + m_v(0)e^{(-t/\tau_3)}}{m_l(0) + m_v(0)} U_l(0) + \frac{m_v(0)(1 - e^{(-t/\tau_3)})}{m_l(0) + m_v(0)} U_v(0) \quad (5.67)$$

$$U_v(t) = \frac{m_l(0)(1 - e^{(-t/\tau_3)})}{m_l(0) + m_v(0)} U_l(0) + \frac{m_l(0)e^{(-t/\tau_3)} + m_v(0)}{m_l(0) + m_v(0)} U_v(0) \quad (5.68)$$

On peut vérifier que la quantité de mouvement totale est également conservée. Les équations portant sur les énergies totales phasiques peuvent être reformulées en énergie interne :

$$\partial_t (m_l e_l) = \mathcal{B}(U_v - U_l)$$

et

$$\partial_t (m_v e_v) = 0$$

Les seconds membres de ces deux équations sont explicitement connus grâce aux expressions (5.67) et (5.68), et sont intégrables. On trouve :

$$(m_l e_l)(t) = (m_l e_l)(0) + \frac{m_l(0)m_v(0)}{m_l(0) + m_v(0)} \frac{(U_l(0) - U_v(0))^2}{2} (1 - e^{(-2t/\tau_3)}) \quad (5.69)$$

$$(m_v e_v)(t) = (m_v e_v)(0) \quad (5.70)$$

Ces solutions permettent de conserver l'énergie totale, c'est-à-dire que l'on a :

$$(m_l e_l + m_l \frac{U_l^2}{2})(t) + (m_v e_v + m_v \frac{U_v^2}{2})(t) = (m_l e_l + m_l \frac{U_l^2}{2})(0) + (m_v e_v + m_v \frac{U_v^2}{2})(0)$$

La mise à jour de la variable W est réalisée en utilisant les solutions (5.64), (5.65), (5.66), (5.67), (5.68), (5.69) et (5.70) au temps $t = \Delta t$ et en prenant comme condition initiale ($t = 0$) les valeurs de W^n .

Remarque. *On a vu que les masses partielles étaient positives ainsi que les titres. L'énergie interne vapeur $m_v e_v$ est trivialement positive, et comme par définition τ_3 est positif, l'énergie interne liquide $m_l e_l$ est aussi positive.*

Remarque. *La méthode proposée ci-dessus pour l'intégration numérique du terme de trainée est valable pour toute loi d'état.*

5.10.3 Intégration numérique du terme de transfert d'énergie

Il s'agit maintenant de traiter le terme source \mathcal{C} qui ne porte que sur les énergies totales :

$$\begin{cases} \partial_t(\alpha_l) = 0 \\ \partial_t(m_l) = 0 \\ \partial_t(m_l U_l) = 0 \\ \partial_t(\alpha_l E_l) = \mathcal{C} \\ \partial_t(m_v) = 0 \\ \partial_t(m_v U_v) = 0 \\ \partial_t(\alpha_v E_v) = -\mathcal{C} \end{cases} \quad (5.71)$$

où le terme \mathcal{C} est :

$$\mathcal{C} = (\tau_4)^{-1} \frac{m_l C_{V,l} m_v C_{V,v}}{m_l C_{V,l} + m_v C_{V,v}} (T_v - T_l)$$

Les première, deuxième, troisième, cinquième et sixième équations du système (5.71) ont pour solutions :

$$\alpha_l(t) = \alpha_l(0) \quad (5.72)$$

$$m_l(t) = m_l(0) \quad (5.73)$$

$$m_v(t) = m_v(0) \quad (5.74)$$

$$U_l(t) = U_l(0) \quad (5.75)$$

$$U_v(t) = U_v(0) \quad (5.76)$$

Nous nous plaçons maintenant dans le cadre de lois d'états du type gaz raides, la relation liant la température phasique à l'énergie interne phasique est (on rappelle que $C_{V,\phi}$ et $P_{\infty,\phi}$ sont des constantes) :

$$\rho_\phi e_\phi = \rho_\phi C_{V,\phi} T_\phi + P_{\infty,\phi} \quad \text{pour } \phi = l, v$$

Les quatrième et septième équations du système (5.71) donnent donc les deux équations aux dérivées ordinaires linéaires couplées :

$$\begin{cases} \partial_t(T_l) = (\tau_4)^{-1} \frac{m_v(0)C_{V,v}}{m_l(0)C_{V,l} + m_v(0)C_{V,v}} (T_v - T_l) \\ \partial_t(T_v) = -(\tau_4)^{-1} \frac{m_l(0)C_{V,l}}{m_l(0)C_{V,l} + m_v(0)C_{V,v}} (T_v - T_l) \end{cases} \quad (5.77)$$

Les températures phasiques sont donc :

$$T_l(t) = T_l(0) + \frac{m_v(0)C_{V,v}}{m_l(0)C_{V,l} + m_v(0)C_{V,v}} (T_v(0) - T_l(0))(1 - e^{(-t/\tau_4)}) \quad (5.78)$$

$$T_v(t) = T_v(0) - \frac{m_l(0)C_{V,l}}{m_l(0)C_{V,l} + m_v(0)C_{V,v}} (T_v(0) - T_l(0))(1 - e^{(-t/\tau_4)}) \quad (5.79)$$

La température à l'équilibre $T_{eq} = \lim_{t \rightarrow \infty} T_l(t) = \lim_{t \rightarrow \infty} T_v(t)$ sera donc admissible :

$$T_{eq} = \frac{m_l(0)C_{V,l}T_l(0) + m_v(0)C_{V,v}T_v(0)}{m_l(0)C_{V,l} + m_v(0)C_{V,v}}$$

Ce qui fournit les formules pour les énergies internes phasiques :

$$(m_l e_l)(t) = (m_l e_l)(0) + \frac{m_v(0)C_{V,l}m_l(0)C_{V,v}}{m_l(0)C_{V,l} + m_v(0)C_{V,v}}(T_v(0) - T_l(0))(1 - e^{(-t/\tau_4)}) \quad (5.80)$$

$$(m_v e_v)(t) = (m_v e_v)(0) - \frac{m_v(0)C_{V,l}m_l(0)C_{V,v}}{m_l(0)C_{V,l} + m_v(0)C_{V,v}}(T_v(0) - T_l(0))(1 - e^{(-t/\tau_4)}) \quad (5.81)$$

On vérifie aisément que la somme des énergies phasiques est conservée, c'est-à-dire :

$$(m_l e_l)(t) + (m_v e_v)(t) = (m_l e_l)(0) + (m_v e_v)(0)$$

Ce qui grâce aux équations (5.73)-(5.76) implique la conservation de l'énergie totale du système.

Si on fait l'hypothèse que les énergies internes phasiques sont positives à $t = 0$, $(m_l e_l)^n > 0$ et $(m_v e_v)^n > 0$, le pas de temps Δt doit vérifier une condition pour que les énergies internes restent positives :

- si $(T_v - T_l)^n > 0$, alors $(m_l e_l)^{n+1}$ est inconditionnellement positive; afin que $(m_v e_v)^{n+1}$ soit positive, Δt doit vérifier :

$$\Delta t < -\tau_4 \ln \left(1 - \frac{(m_l^n C_{V,l} + m_v^n C_{V,v})}{m_l^n C_{V,l} C_{V,v} (T_v^n - T_l^n)} e_v^n \right)$$

sauf si :

$$1 - \frac{(m_l^n C_{V,l} + m_v^n C_{V,v})}{m_l^n C_{V,l} C_{V,v} (T_v^n - T_l^n)} e_v^n < 0$$

auquel cas il n'y a pas de contrainte sur le pas de temps.

- si $(T_v - T_l)^n < 0$, alors $(m_v e_v)^{n+1}$ est inconditionnellement positive; pour que $(m_l e_l)^{n+1}$ soit positive, Δt doit vérifier :

$$\Delta t < -\tau_4 \ln \left(1 + \frac{(m_l^n C_{V,l} + m_v^n C_{V,v})}{m_v^n C_{V,l} C_{V,v} (T_v^n - T_l^n)} e_l^n \right)$$

sauf si :

$$1 + \frac{(m_l^n C_{V,l} + m_v^n C_{V,v})}{m_v^n C_{V,l} C_{V,v} (T_v^n - T_l^n)} e_l^n < 0$$

auquel cas il n'y a pas de contrainte sur le pas de temps.

- Dans le cas particulier où $T_v^n = T_l^n$, la positivité est trivialement vérifiée.

Chapitre 6

Conclusion

Parmi le peu de travaux existant sur le couplage instationnaire de modèles, très peu concernent le couplage interfacial instationnaire. Certaines équipes (par exemple le CCSM à l'UCAR ou le CITS à Stanford) travaillent sur des coupleurs de modèles basés sur des reconstructions de données par interpolation et sur le calcul de flux de couplage défini de façon analytique. Les travaux présentés dans cette thèse sont quant à eux basés sur une autre approche ; l'idée est d'utiliser l'information contenue dans les modèles à coupler pour calculer les flux de couplage. Ceci est actuellement réalisé de deux manières différentes.

Le groupe de travail sur le couplage interfacial de l'Université de Jussieu-Paris VI s'est attaché au développement de la méthode dite de couplage par état (voir notamment [38],[39]). Le flux de couplage destiné à un modèle est calculé sur la base de la résolution du problème de Riemann associé au système de ce modèle et aux états droit et gauche se trouvant de part et d'autre de l'interface de couplage. Un des avantages de cette technique est de pouvoir choisir d'assurer la continuité de certaines grandeurs à la traversée de l'interface de couplage en appliquant un changement de variables approprié aux états de part et d'autre de l'interface de couplage.

L'approche retenue dans ce travail de thèse a été basée dans un premier temps sur les travaux de Leroux et Greenberg (voir par exemple [44]) et a par la suite été complétée par des techniques de relaxation instantanée. Dans les deux cas, les flux de couplage sont calculés à partir d'un unique problème de Riemann. Celui-ci est basé sur le système d'équations d'un modèle père reprenant l'intégralité de l'information contenue dans les modèles à coupler. Ce modèle père est donc utilisé de deux manières : la partie convective du système d'équations permet de calculer les flux de couplage ; une méthode de relaxation instantanée permet, si cela est nécessaire, de calculer des approximations numériques de chacun des modèles à coupler (voir en particulier les chapitres 4 et 5).

L'ensemble de ces travaux a permis de mettre en lumière plusieurs points importants liés aux modèles existants ainsi qu'à leur couplage.

- (i) Certains modèles utilisés dans l'industrie présentent des lacunes du point de vue du cadre actuel des mathématiques des systèmes de lois de conservation. La définition des termes sources n'est pas toujours en adéquation avec la notion de dissipation d'entropie ; il s'agit souvent d'un problème de compatibilité entre le terme source et les lois de fermeture thermodynamiques qui entraîne des difficultés dans la définition des solutions choc. L'utilisation du modèle bi-fluide standard, qui n'est pas toujours hyperbolique et dont la structure propre n'est à vrai dire pas

explicitement connue, reste acceptable sur maillage grossier. L'augmentation progressive des capacités de calcul permet de travailler sur des maillages de plus en plus fins, et les lacunes du modèle bi-fluide standard ne pourront plus être masquées par la diffusion numérique. C'est dans cette optique qu'il est intéressant de disposer de nouveaux modèles mieux appropriés à la simulation numérique sur maillage fin.

- (ii) Dans les travaux des chapitres 4 et 5 des modèles proches ont été couplés. D'une certaine manière la méthode de couplage mise en oeuvre permet de mesurer la différence entre les modèles. Cela est particulièrement sensible au chapitre 4 ; en faisant tendre la constante de temps du transfert de masse vers zéro, on peut "faire tendre" le modèle HRM vers le modèle HEM. Pour des constantes de temps grandes les deux modèles fournissent des réponses complètement différentes et on est alors en droit de se demander si leur couplage a encore un sens. Le même phénomène est observable au chapitre 5, avec comme principale différence le fait que le modèle bi-fluide standard ne coïncide pas avec le modèle HRM quand les vitesses phasiques sont équilibrées (à ce sujet voir l'étude de sensibilité de la solution couplée par rapport à la constante de temps du terme de trainée).
- (iii) Dans certains cas des degrés de liberté liés à la physique sont apparus. Un premier point apparaît dans [49] où il est nécessaire de définir les pertes de charge. Ce sont des données qui devraient être calibrées par des études physiques et expérimentales. D'autre part, la méthode employée par le groupe de travail de l'Université de Jussieu-Paris VI permet d'assurer la continuité de certaines grandeurs physiques, la question étant de connaître la pertinence du choix de telle ou telle variable.

En ce qui concerne la simulation et le couplage de modèles, les techniques de relaxation semblent très prometteuses. En effet on pourrait envisager d'utiliser un modèle père relativement général afin de simuler et de coupler entre eux tout un ensemble de modèles "fils". On pourrait par exemple envisager d'utiliser un modèle père basé sur le modèle bi-fluide à deux pressions pour simuler et coupler les modèles suivants : modèle bi-fluide à deux pressions (sept équations), modèle bi-fluide standard (six équations), modèle à cinq équations, modèles de type HRM (quatre équations), modèles de type HEM (trois équations). Un unique code permettrait ainsi de simuler plusieurs modèles et d'en assurer le couplage. Un autre avantage de cette technique est que la compatibilité entre les différents modèles est implicitement assurée. Un premier inconvénient observé vient du fait que, sur un même cas test, les profils d'ondes d'une solution obtenue par une technique de relaxation sont plus diffusés que ceux de la solution obtenue par une simulation directe. L'inconvénient principal réside dans l'inconnu qu'il y a autour de la manière dont les modèles fils héritent des propriétés thermodynamiques du modèle père. Dans le cas du chapitre 5, les lois thermodynamiques du modèle à six équations sont parfaitement connues ; en revanche nous ne sommes pas en mesure d'explicitement la loi d'état du modèle HRM simulé.

Un cas industriel de couplage entre le code NEPTUNE_CFD et un code basé sur un modèle HRM a été réalisé en adaptant les techniques retenues pour les cas de couplage des chapitres 3 et 5. Les résultats ainsi obtenus sont très encourageants et la méthode s'est avérée stable.

Annexe A

Rigid wall boundary conditions for Euler system

We are interested here in computing the exact Godunov flux for rigid wall boundary conditions for the Euler system with the stiffened gas EOS.

We consider here the Euler system:

$$\partial_t (\rho) + \partial_x ((\rho u)) = 0 \quad (\text{A.1})$$

$$\partial_t ((\rho u)) + \partial_x ((\rho u^2 + P)) = 0 \quad (\text{A.2})$$

$$\partial_t (E) + \partial_x ((u(E + P))) = 0 \quad (\text{A.3})$$

with the definition,

$$E = \rho \epsilon + \rho \frac{u^2}{2} \quad (\text{A.4})$$

and the stiffened gas equation of state:

$$(\gamma - 1)\rho \epsilon = P + \gamma P_{inf} \quad (\text{A.5})$$

A classical method to compute the rigid wall boundary conditions is the mirror state technique. If in the near wall cell the variables are (ρ_L, U_L, P_L) then the virtual right cell is defined with variables $(\rho_R = \rho_L, U_R = -U_L, P_R = P_L)$. When solving the Riemann problem associated with ((A.1)-(A.3)) and ((A.4),(A.5)) with the above left and right states we find that the solution for u is always $u = 0$. Then the exact Godunov flux is:

$$F^{God} = (0, P^*, 0)$$

with the following definition of P^* :

– If $U_L < 0$, double rarefaction waves configuration :

The vacuum numerically occurs if $|U_L| > 2C^2/(\gamma - 1)$ and then we have:

$$\rho^* = 0 \quad \text{and} \quad P^* = -\gamma P_{inf}$$

otherwise,

$$P^* + P_{inf} = (P_L + P_{inf}) \left(1 + M \frac{\gamma - 1}{2} \right)^{\frac{2\gamma}{\gamma - 1}}$$

– If $U_L > 0$, double shock waves configuration,

$$P^* = P_L \left(1 + \frac{\gamma(\gamma+1)}{4} RM^2 \right) + P_L MR \gamma \left(1 + \frac{(\gamma+1)^2}{16} RM^2 \right)^{1/2}$$

We have used the following notation, the celerity of sound in the left cell:

$$C = \sqrt{\gamma \frac{P_L + P_{inf}}{\rho_L}} = \sqrt{\gamma \frac{P_R + P_{inf}}{\rho_R}}$$

the Mach number M in the left cell:

$$M = \frac{U_L}{C_L} = -\frac{U_R}{C_R}$$

and the parameter,

$$R = \frac{P_L + P_{inf}}{P_L} = \frac{P_R + P_{inf}}{P_R}$$

Annexe B

Coupling two and one dimensional Euler models

The main part of this chapter was devoted to the study of different ways to couple the one- and two-dimensional isentropic Euler systems. In fact these systems are not those used in the Neptune project and in the nuclear community. More realistic codes are based on model that possess (at least) an energy equation. This equation involves the transverse velocity, so that one can expect that the work presented above does not apply anymore. We will prove in the following that the proposed methods still apply when considering some "complicated models" such as a HRM model or a simple model for the turbulence.

B.1 Models to be coupled

B.1.1 Presentation of the Euler system

The vacuum occurrence is not in our scope, we will assume that the density always remains positive. The present section is a short presentation of the Euler models, some complementary informations can be found for instance in [37].

The one-dimensional Euler system reads:

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \tag{B.1}$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \tag{B.2}$$

$$\partial_t (E_1) + \partial_x (u(E_1 + P)) = 0 \tag{B.3}$$

where u , ρ , E_1 and P respectively stand for the velocity, the density, the total energy and the pressure. The system is completed by a relation that relies the pressure and the density to the internal energy $e_1(P, \rho)$, which one appears in the total energy definition:

$$E_1 = \rho e_1(P, \rho) + \rho \frac{u^2}{2}$$

The system (B.1)-(B.3) is hyperbolic if and only if:

$$(\partial_P (e_1))^{-1} \left(\frac{P}{\rho} - \rho \partial_\rho (e_1) \right) > 0$$

The two-dimensional Euler system reads:

$$\partial_t (\rho) + \partial_x (\rho u) + \partial_y (\rho v) = 0 \quad (\text{B.4})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) + \partial_y (\rho uv) = 0 \quad (\text{B.5})$$

$$\partial_t (\rho v) + \partial_x (\rho uv) + \partial_y (\rho v^2 + P) = 0 \quad (\text{B.6})$$

$$\partial_t (E_2) + \partial_x (u(E_2 + P)) + \partial_y (v(E_2 + P)) = 0 \quad (\text{B.7})$$

where v is the transverse velocity and E_2 the total energy which is written here as:

$$E_2 = \rho e_2(P, \rho) + \rho \left(\frac{u^2}{2} + \frac{v^2}{2} \right)$$

The system must be completed writing a relation that relies the pressure and the density to the internal energy $e_2(P, \rho)$, moreover it is hyperbolic if and only if:

$$(\partial_P (e_2))^{-1} \left(\frac{P}{\rho} - \rho \partial_\rho (e_2) \right) > 0$$

B.1.2 The left and right systems of equations

Without loss of generality we assume that the interface of coupling is along the y -axis at $x = 0$. The two sets of equations (B.1)-(B.3) and (B.4)-(B.7) thus respectively read (B.8)-(B.10) and (B.11)-(B.14).

On the left side of the interface we consider the one-dimensional Euler system:

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.8})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.9})$$

$$\partial_t (E_1) + \partial_x (u(E_1 + P)) = 0 \quad (\text{B.10})$$

On the right side of the interface we consider the two-dimensional Euler system:

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.11})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.12})$$

$$\partial_t (E_2) + \partial_x (u(E_2 + P)) = 0 \quad (\text{B.13})$$

$$\partial_t (\rho v) + \partial_x (\rho uv) = 0 \quad (\text{B.14})$$

In the following we will consider that the two models have the same equation of state, that is (the case of different EOS is shortly discussed at the end of the present appendix):

$$e_1(P, \rho) = e_2(P, \rho) = e(P, \rho), \quad \forall (P, \rho)$$

B.2 Rewriting the two-dimensional Euler system

At the first sight, coupling the one- and two-dimensional Euler systems seems to be a different problem than for the isentropic case. Indeed a new difficulty appears, the equations (B.10) and

(B.13) are different and this one involves the variable v . We thus want to write the system (B.11)-(B.14) in terms of the system (B.8)-(B.10). First of all we note that the total energy E_2 can be expressed as:

$$E_2 = E_1 + \rho \frac{v^2}{2}$$

Considering a Riemann problem, the solution of the system (B.8)-(B.10) and (B.11)-(B.14) are piecewise regular functions (see [37] for instance). We thus have to distinguish the case of regular solutions and the case of the discontinuities that occurs in shock waves and contact discontinuity waves.

B.2.1 The regular solutions

We first focus on regular solutions that occurs for rarefaction waves and for the intermediate states. Using the mass equation (B.11) and the transverse momentum equation (B.14) we find the following equation for the transverse kinetic energy:

$$\partial_t \left(\rho \frac{v^2}{2} \right) + \partial_x \left(\rho u \frac{v^2}{2} \right) = 0$$

Hence we obviously have:

$$\partial_t (E_2) + \partial_x (u(E_2 + P)) = 0 \iff \partial_t (E_1) + \partial_x (u(E_1 + P)) = 0$$

B.2.2 The shock solutions

Let us focus now on the discontinuities. They are governed by the classical Rankine-Hugoniot relations. For a shock with the speed σ , the Rankine-Hugoniot relation for the equations (B.11) and (B.14) are respectively:

$$-\sigma[\rho] + [\rho u] = 0 \tag{B.15}$$

$$-\sigma[\rho v] + [\rho uv] = 0 \tag{B.16}$$

For a variable X we use the notation $[X] = X^+ - X^-$ and $\overline{X} = \frac{X^+ + X^-}{2}$; where X^+ (reps. X^-) is the value on the right (resp. left) side of the discontinuity. Combining the jump relations (B.15) and (B.16) we can obtain the relation:

$$(-\sigma\overline{\rho} + \overline{\rho u})[v] = 0 \tag{B.17}$$

The Rankine-Hugoniot relation for the total energy equation (B.13) can be written:

$$-\sigma[E_1] + [u(E_1 + P)] + \left(-\sigma \left[\rho \frac{v^2}{2} \right] + \left[\rho u \frac{v^2}{2} \right] \right) = 0$$

and because of the relation (B.17) we have:

$$-\sigma \left[\rho \frac{v^2}{2} \right] + \left[\rho u \frac{v^2}{2} \right] = (-\sigma\overline{\rho} + \overline{\rho u})[v]\overline{v} = 0$$

Hence we finally get the following equivalence:

$$-\sigma[E_2] + [u(E_2 + P)] = 0 \iff -\sigma[E_1] + [u(E_1 + P)] = 0$$

B.2.3 Consequence for the two-dimensional Euler system

Finally the set of equations (B.11)-(B.14) is equivalent to the set of equations (B.18)-(B.21), either for regular solutions and for discontinuities:

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.18})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.19})$$

$$\partial_t (E_1) + \partial_x (u(E_1 + P)) = 0 \quad (\text{B.20})$$

$$\partial_t (\rho v) + \partial_x (\rho u v) = 0 \quad (\text{B.21})$$

The keystone of this rewriting is that -thanks to the mass equation- the convection of the transverse kinetic energy $\rho \frac{v^2}{2}$ is exactly the same as for transverse momentum ρv .

An important point to be quoted is that the subset of equations (B.18)-(B.20) does not depend on v . It is the same set of equations than (B.8)-(B.10). We can then apply the methods of flux coupling proposed for the isentropic Euler model.

B.3 An interface model for flux coupling

The (NSC) condition presented above keeps its importance in the present case. Hence an interface model is admissible if and only if it respects this condition. We propose herein two models. A non conservative model the Jacobian matrix of which is the a weighted average of the left and right Jacobian matrixes. A conservative model the flux of which is a weighted average of the left and right fluxes.

B.3.1 A non conservative admissible interface model

Following [44] we introduce here a new variable which distinguishes the two domains and does not depend on time t ,

$$z(x,y,t) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases}$$

We now consider the following interface model:

$$\partial_t (z) = 0 \quad (\text{B.22})$$

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.23})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.24})$$

$$\partial_t (E_1) + \partial_x (u(E_1 + P)) = 0 \quad (\text{B.25})$$

$$\partial_t (v) + zu\partial_x (v) = 0 \quad (\text{B.26})$$

This system can not be written in conservative form because of the non-conservative product [63] $zu\partial_x (v)$. In fact the solution of the Riemann problem is classical for (B.22)-(B.25) (unless resonance phenomena occurs), but we have to propose a way to solve (B.26). This is achieved using the same idea as for the isentropic case.

In terms of the variable $(z, \rho, u, P, v)^\top$, the eigenvalues and eigenvectors are:

$$\begin{aligned}\lambda_1 &= 0, & r_1^\top &= (1, 0, 0, 0, 0) \\ \lambda_2 &= u - c, & r_2^\top &= (0, \rho, -c, \rho c^2, 0) \\ \lambda_3 &= u, & r_3^\top &= (0, 1, 0, 0, 0) \\ \lambda_4 &= u + c, & r_4^\top &= (0, \rho, c, \rho c^2, 0) \\ \lambda_5 &= zu, & r_5^\top &= (0, 0, 0, 0, 1)\end{aligned}$$

In the following v_R denotes the value of the velocity of the right state for the Riemann problem and we set $\lambda_3 = u^*$. For v we choose the same solution as for the non conservative admissible interface model proposed for the isentropic Euler model that is:

$$\begin{aligned}v(x/t = 0^-) &= 0 \\ v(x/t = 0^+) &= \begin{cases} 0 & \text{if } u^* > 0 \\ v_R & \text{if } u^* < 0 \end{cases}\end{aligned}$$

The solution at $x/t = 0^-$ (resp. $x/t = 0^+$) allows the computation of the flux F^- (resp. F^+) at $x/t = 0^-$ (resp. $x/t = 0^+$). This numerical flux is passed as a boundary condition to the left (resp. right) code. The notation $\Phi(x/t = 0^+) = \Phi^+$ and $\Phi(x/t = 0^-) = \Phi^-$ will be used to clarify the formulae. The numerical fluxes are:

$$F^- = \begin{pmatrix} (\rho u)^- \\ (\rho u^2 + P)^- \\ (u(E_1 + P))^- \\ 0 \end{pmatrix}, \quad F^+ = \begin{pmatrix} (\rho u)^+ \\ (\rho u^2 + P)^+ \\ (u(E_2 + P))^+ \\ (\rho u v)^+ \end{pmatrix}$$

Note that because of the independence of the subset of equations (B.23)-(B.25) with respect to the variables z and v the corresponding flux components are continuous at $x/t = 0$, that is:

$$\begin{aligned}(\rho u)^- &= (\rho u)^+ = (\rho u)^* \\ (\rho u^2 + P)^- &= (\rho u^2 + P)^+ = (\rho u^2 + P)^* \\ (u(E_1 + P))^- &= (u(E_1 + P))^+ = (u(E_1 + P))^*\end{aligned}$$

The fluxes F^+ and F^- can thus expressed as:

$$F^- = \begin{pmatrix} (\rho u)^* \\ (\rho u^2 + P)^* \\ (u(E_1 + P))^* \\ 0 \end{pmatrix}, \quad F^+ = F^- + \begin{pmatrix} 0 \\ 0 \\ \frac{(\rho u)^*}{2} (v^+)^2 \\ (\rho u)^* v^+ \end{pmatrix}$$

Obviously the coupling method respect the (NSC) condition and is not conservative. In fact the density and the axial momentum will be preserved whereas the transverse momentum and the total

energy will not be preserved.

Remark 22 *We obtain the same discrete fluxes using the Godlewski-Raviart method using the left and right fluxes:*

$$f_L = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ u(E_1 + P) \\ 0 \end{pmatrix} \text{ and } f_R = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ u(E_2 + P) \\ \rho uv \end{pmatrix}$$

B.3.2 A conservative admissible interface model

We introduce now a conservative interface model that respect the (NSC) condition. This model is exactly the counterpart of the conservative model proposed for the isentropic case. The governing equations are:

$$\partial_t(z) = 0 \tag{B.27}$$

$$\partial_t(\rho) + \partial_x(\rho u) = 0 \tag{B.28}$$

$$\partial_t(\rho u) + \partial_x(\rho u^2 + P) = 0 \tag{B.29}$$

$$\partial_t(E_1) + \partial_x(u(E_1 + P)) = 0 \tag{B.30}$$

$$\partial_t(\rho v) + \partial_x(zu\rho v) = 0 \tag{B.31}$$

The solution of a Riemann problem with a left and right states fulfilling:

$$\begin{aligned} v_L &= 0 \\ z_L &= 0 \quad \text{and} \quad z_R = 1 \end{aligned}$$

is obtained using the same idea than for the isentropic Euler coupling case. This leads to the following transverse fluxes for momentum:

$$(\rho uv)(x/t = 0^-) = (\rho uv)(x/t = 0^+) = 0$$

Hence the left and right fluxes are:

$$F^- = F^+ = \begin{pmatrix} (\rho u)^* \\ (\rho u^2 + P)^* \\ (u(E_1 + P))^* \\ 0 \end{pmatrix}$$

This model thus fulfil the (NSC) condition and since $F^- = F^+$ this coupling method is conservative.

B.4 Numerical results

We use the above methods to simulate the Euler model with perfect gas EOS, that is:

$$(\gamma - 1)\rho e(P, \rho) = P$$

The test case configuration is the same as the one described for the isentropic Euler systems. We choose to present the results obtained for the gas simulation, that is $\gamma = 1.4$. The initial conditions are:

$$\begin{aligned}\rho(x,y;t=0) &= \begin{cases} 0.5 & \text{if } y > x - 0.15 \\ 1.0 & \text{else.} \end{cases} \\ P(x,y;t=0) &= \begin{cases} 10^4 & \text{if } y > x - 0.15 \\ 10^5 & \text{else.} \end{cases} \\ u(x,y;t=0) &= v(x,y;t=0) = 0.0\end{aligned}$$

The interface is located in $x = 0$ (i.e. at the connection between the pipe and the tank). All interfacial fluxes are computed using a VFRoe-ncv [16] scheme using the variable $(\rho, u, P, v)^\top$ and the time steps are computed to respect a CFL of 1/2.

The density and the transverse momentum are plotted on the line $y = 0$ with respect to x . The so-called two-dimensional reference solution is the computation obtained using the two-dimensional Euler model on the whole domain with the mesh refined in all the direction. The results are computed on the finest meshes. For conservative admissible model the overshoot of the transverse velocity produced a bluff-body phenomenon in the beginning of the pipe that make the computation stop (the density in at least one cell becomes negative), results are plotted at the last time step before this blow-out.

Moreover we observe that comparatively to the conservative admissible model (represented by squares on figures), the non conservative admissible model (represented by circles on figures) is much closer from the reference solution (represented by crosses on figure) near the coupling interface.

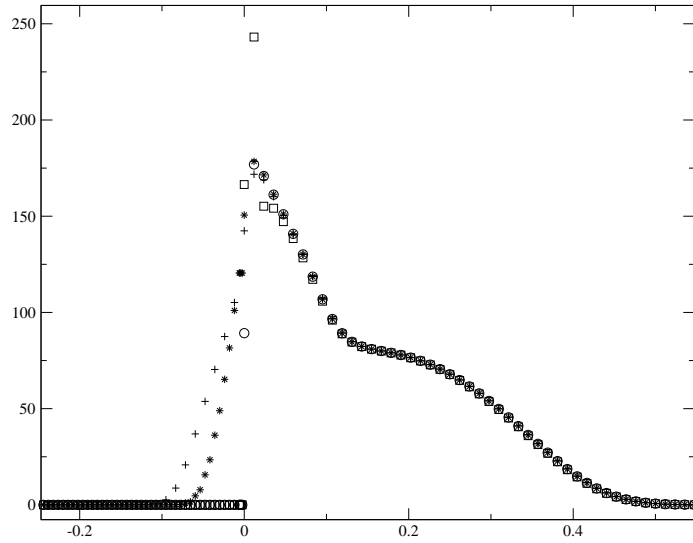


FIG. B.1 – Solution for the transverse momentum on the line $y=0$. Crosses stand for the two-dimensional reference solution, stars stand for the natural interface model (which does not respect the (NSC)), circles stand for the non conservative admissible interface model and squares stand for the conservative admissible interface model.

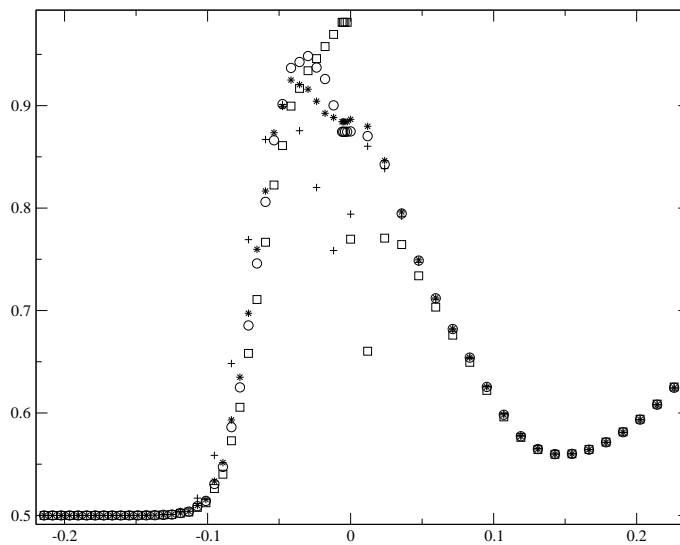


FIG. B.2 – Solution for the density on the line $y=0$. Crosses stand for the two-dimensional reference solution, stars stand for the natural interface model (which does not respect the (NSC)), circles stand for the non conservative admissible interface model and squares stand for the conservative admissible interface model.

B.5 Some remarks

B.5.1 Other realistic models

The above approach can be extended to systems based on the Euler equations: a Homogeneous Relaxed Model (HRM) or a simple model dealing with the turbulence for instance. We still assume herein that the coupling interface is along the y -axis and that the equation of states are the same for the one- and two-dimensional systems. For the sake of brevity, we will just give the manner of rewriting the two-dimensional system.

A Homogeneous Relaxed Model

HRM models are widely used in two-phase simulation for nuclear power plant. Omitting source terms and drift effect, the governing equations of a HRM model are:

$$\partial_t (\rho\alpha) + \partial_x (\rho u\alpha) = 0 \quad (\text{B.32})$$

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.33})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.34})$$

$$\partial_t (E_2) + \partial_x (u(E_2 + P)) = 0 \quad (\text{B.35})$$

$$\partial_t (\rho v) + \partial_x (\rho uv) = 0 \quad (\text{B.36})$$

with $E_2 = \rho e(P, \rho, \alpha) + \rho(\frac{u^2}{2} + \frac{v^2}{2})$. The variables ρ , u , v , P and e respectively stand for the mean density, the mean axial velocity, the mean transverse velocity, the pressure and the internal energy of the mixture. In terms of $E_1 = \rho e(P, \rho, \alpha) + \rho\frac{u^2}{2}$, the two-dimensional HRM system above is equivalent to:

$$\partial_t (\rho\alpha) + \partial_x (\rho u\alpha) = 0 \quad (\text{B.37})$$

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.38})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.39})$$

$$\partial_t (E_1) + \partial_x (u(E_1 + P)) = 0 \quad (\text{B.40})$$

$$\partial_t (\rho v) + \partial_x (\rho uv) = 0 \quad (\text{B.41})$$

A simple model of turbulence

The governing equations of a simple model of turbulence are:

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.42})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.43})$$

$$\partial_t (E_2) + \partial_x \left(u(E_2 + P + \frac{2}{3}K) \right) = 0 \quad (\text{B.44})$$

$$\partial_t (K) + \partial_x (uK) + \frac{2}{3}K\partial_x (u) = 0 \quad (\text{B.45})$$

$$\partial_t (\rho v) + \partial_x (\rho uv) = 0 \quad (\text{B.46})$$

With the closure $E_2 = \rho e_2(P, \rho) + \rho(\frac{u^2}{2} + \frac{v^2}{2}) + K$. Where here ρ , u , v , P , K and e_2 are respectively the mean density, the mean axial velocity, the mean transverse velocity, the pressure, the mean internal

energy and the turbulent kinetic energy. In terms of $E_1 = \rho e(P, \rho) + \rho \frac{u^2}{2} + K$ the two-dimensional above system can be written:

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.47})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.48})$$

$$\partial_t (E_1) + \partial_x \left(u(E_1 + P + \frac{2}{3}K) \right) = 0 \quad (\text{B.49})$$

$$\partial_t (K) + \partial_x (uK) + \frac{2}{3}K \partial_x (u) = 0 \quad (\text{B.50})$$

$$\partial_t (\rho v) + \partial_x (\rho uv) = 0 \quad (\text{B.51})$$

B.5.2 Different forms for internal energy

We focus here again on the systems (B.11)-(B.14) and (B.8)-(B.10) but we do not make the assumption that the internal energies are the same that is we have: $e_1(P, \rho) \neq e_2(P, \rho)$. Let us define E_2^* as:

$$E_2^* = E_2 - \rho \frac{v^2}{2} = \rho e_2(P, \rho) + \rho \frac{u^2}{2}$$

The two-dimensional Euler system (B.11)-(B.14) is equivalent to the following system:

$$\partial_t (\rho) + \partial_x (\rho u) = 0 \quad (\text{B.52})$$

$$\partial_t (\rho u) + \partial_x (\rho u^2 + P) = 0 \quad (\text{B.53})$$

$$\partial_t (E_2^*) + \partial_x (u(E_2^* + P)) = 0 \quad (\text{B.54})$$

$$\partial_t (\rho v) + \partial_x (\rho uv) = 0 \quad (\text{B.55})$$

Hence in the problem of coupling the system (B.52)-(B.55) to the system (B.8)-(B.10) we can distinguish two independent coupling problems:

- (i) to couple two Euler models with different EOS, involving the two subsets of equations (B.52)-(B.54) and (B.8)-(B.10)
- (ii) to couple one- and two-dimensional Euler models, involving the equations (B.55) and the fictitious equation $\partial_t (\rho v) = 0$.

The item (i) has been addressed in [4], while we have proposed a method for the second item (ii).

Annexe C

A relaxation method to compute two-fluid models

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Abstract : We describe in this paper a tool to compute approximate solutions of standard two-fluid models with an equilibrium pressure assumption. The basic approach takes its grounds in the two-fluid two-pressure formalism, and takes advantage of the relaxation techniques. The method may be used to compute either the single pressure or the two-pressure model, depending on the size of mesh which is used. It is also shown on the basis of a simple numerical experiment that the local equilibrium assumption may lead to a blow-up of the numerical solution on fine meshes, even if one accounts for drag stabilizing effects.

C.1 Introduction

There has been a wide debate over the past thirty years in the two-phase flow community, which concerns the potential loss of hyperbolicity of standard two-fluid models, and its consequences in terms of industrial predictions of two-phase flows. A first idea that emerged a long time ago is the following: even if the standard two-fluid model may lead in some test cases to an ill-posed initial value problem, this will never have negative consequences since one uses rather coarse meshes and meanwhile the upwinding flavour will guarantee enough stability to compensate emerging inner instability of the set of PDE. Actually, this might make sense provided that we deal with discrete models, and not with continuous models. A second point which is also emphasised is that some (expected small) interfacial transfer terms in the momentum equation (namely $\beta \partial_x(\alpha)$) may become predominant in "dangerous" situations. This was first pointed out by Stuhmiller a long time ago when focusing on *incompressible media*, and more recently in the nuclear community. An annoying point is that this term only enlarges the domain of hyperbolicity ([79]), but in such a way that it cannot exactly recover the whole domain including all physically admissible states.

An alternative way to compute two-fluid models has emerged quite recently, which takes its grounds on the two-fluid two-pressure approach. One of the main advantages of the latter formalism is that it guarantees hyperbolicity for all admissible states (that is physical states with positive volume fractions, positive mass fractions and internal energies). However, many workers in the two-fluid community still seem to feel reluctant using these. The main objective here is to give a common framework which might unify both approaches, and meanwhile inherit of mathematical properties of the two-pressure closures.

The basic idea in this work is thus to take advantage of the structure of two-fluid two-pressure models to provide approximations on coarse meshes of standard two-fluid models. Actually, we show how to construct a simple numerical method which ensures that the maximum principle for the void fraction holds, and either leads to the prediction of the two-fluid two-pressure approach when using finite time relaxation, or to the standard two-fluid model when using zero relaxation time. Both rely on a control of the entropy inequality. We will also show, on the basis of a particular test case issuing from the literature, that the second algorithm hides deficiencies on coarse meshes which are nonetheless naturally retrieved when applying for hudge mesh refinement. This expected result is meaningful, and has already been pointed out some time ago in [22] in the framework of gas flow highly loaded with particles.

The whole algorithm is grounded on relaxation schemes. These have become quite popular over the past ten years, mainly because they enable to deal with complex EOS when computing gas dynamics with Euler equations (see [59] and [62] for instance). They are indeed useful to cope with nonlinear EOS, and enable to retrieve similar rates of convergence when compared with more standard exact or approximate Riemann solvers. The application to the frame of two-phase flows also seems very appealing. This has been recently investigated by F. Coquel and co-authors in order to cope with two-phase homogeneous models in industrial situations (see [13], [15], [18], [24], [26], [31]). The presentation of the paper is the following. We first provide the overall algorithm. We afterwards recall some properties of the two-fluid two-pressure model, and of the relaxation step. Schemes which are used to provide approximations within each step are then examined. The basic numerical example which is discussed in this paper is a simple Riemann problem issuing from the

literature. We will focus on the standard two-fluid single pressure model. We briefly recall that this model leads to a blow-up of the computation when stabilizing drag effects are omitted, assuming the mesh is fine enough. We then consider the same initial conditions and account for drag effects with physical drag coefficients. For coarse or not too fine meshes, the numerical solution seems to be physically relevant ; however, the numerical approximation still blows up when one makes a -hudge-mesh refinement. Of course, results obtained with the two-pressure model do not suffer from this deficiency.

C.2 Two-fluid models and main algorithm

We first introduce some classical notations. The subscript $k \in \{1,2\}$ will refer to the phase 1 and 2 respectively. Let U_k , ρ_k and P_k be the velocity, the density and the pressure within phase k . The volume fraction in each phase is denoted by $\alpha_k \in [0,1]$ with $\alpha_1 + \alpha_2 = 1$. The partial masses are $m_k = \alpha_k \rho_k$, and $E_k = \rho_k e_k + \frac{\rho_k U_k^2}{2}$ stands for the total energy of phase k , where the internal energy is noted $e_k = e_k(P_k, \rho_k)$.

C.2.1 The standard two-fluid model

We first briefly recall that the standard two-fluid model (C.1) is a 6–equation model with two mass conservation equations, two momentum equations and two total energy equations.

$$\left\{ \begin{array}{l} \partial_t (m_k) + \partial_x (m_k U_k) = 0 \\ \partial_t (m_k U_k) + \partial_x (m_k U_k^2) + \alpha_k \partial_x (P) \\ = T_k \\ \partial_t (\alpha_k E_k) + \partial_x (\alpha_k U_k (E_k + P)) + P \partial_t (\alpha_k) \\ = T_k V^i \end{array} \right. \quad (\text{C.1})$$

The interfacial momentum transfer T_k in phase k agregates the contributions of the drag force, which is:

$$T_{k,0} = (-1)^k K(W)(U_1 - U_2) \quad (\text{C.2})$$

and the first order differential correction:

$$T_{k,1} = -(P - \pi^i) \partial_x (\alpha_k) \quad (\text{C.3})$$

which vanishes when one assumes that $\pi_i = P$, and contributes to enlarge the hyperbolicity domain when $\pi_i - P = \beta(U_2 - U_1)^2$ (see [78]). It is known from long that the eigenstructure of the convective part of this system can not be analytically exhibited. This lack of information obviously prevents us from building the exact solution of the Riemann problem, and also renders the construction of approximate Riemann solvers very tedious (see [78], [76]). But the most annoying point is that one also knows that some "elliptic" (with respect to time) areas remain, which results in a "blow-up" of the continuous solution, as illustrated in [68] (in other words, the initial boundary value problem becomes locally ill-posed). As a consequence, whatever the (assumed convergent) numerical method is, one expects that the approximate solution will also explode on *sufficiently* small grid sizes. We nonetheless underline that this strange pattern should not be confused with the preservation of the maximum principle for the volume fraction. Actually, regular solutions of the standard two-fluid model, agree with the maximum principle for α_1 , if the velocity fields (and their divergences) remain bounded over finite time intervals (see [20]).

C.2.2 The two-fluid two-pressure model

This one may be written as:

$$\begin{cases} \partial_t (\alpha_1) + V^i \partial_x (\alpha_1) = \lambda(P_1 - P_2) \\ \partial_t (m_k) + \partial_x (m_k U_k) = 0 \\ \partial_t (m_k U_k) + \partial_x (m_k U_k^2 + \alpha_k P_k) - P^i \partial_x (\alpha_k) = T_k \\ \partial_t (\alpha_k E_k) + \partial_x (\alpha_k U_k (E_k + P_k)) + P^i \partial_t (\alpha_k) = T_k V^i \end{cases} \quad (\text{C.4})$$

We will detail afterwards the specific forms of the interface velocity V_i and interface pressure P^i . Setting in a formal way $\lambda = +\infty$ enables to retrieve the previous set associated with the standard two-fluid model.

The interfacial velocity and the interfacial pressure are modelled in a classical way (see [9], [12], [25], [34],[35], [48], [60]):

$$V_i = \mu U_1 + (1 - \mu) U_2 \quad (\text{C.5})$$

where either $\mu(1 - \mu) = 0$ (see [12]), or $\mu = \frac{m_1}{m_1 + m_2}$ (see [25]). Moreover:

$$P^i = \frac{(1 - \mu)a_1 P_1 + \mu a_2 P_2}{(1 - \mu)a_1 + \mu a_2} \quad (\text{C.6})$$

where $a_k = (\partial_{P_k} (e_k(P_k, \rho_k)))^{-1} \partial_{P_k} (Ln(s_k)(P_k, \rho_k))$.

C.2.3 The basic algorithm

Still using all above notations, we may now present the whole computational process between discrete time t^n and t^{n+1} .

It consists in two steps :

- (i) an evolution step,
- (ii) and a relaxation step.

During the evolution step, we compute an approximate solution of the two-fluid two-pressure model, -the basics of which are recalled later on-, *omitting the pressure relaxation terms*. The initial condition in cell i for this evolution step is Z_i^n , where $Z^t = (\alpha_1, m_1, m_2, m_1 U_1, m_2 U_2, \alpha_1 E_1, \alpha_2 E_2)$.

Thus the governing set of equations of the evolution step will be:

$$\begin{cases} \partial_t (\alpha_1) + V^i \partial_x (\alpha_1) = 0 \\ \partial_t (m_k) + \partial_x (m_k U_k) = 0 \\ \partial_t (m_k U_k) + \partial_x (m_k U_k^2) + \partial_x (\alpha_k P_k) - P^i \partial_x (\alpha_k) = T_k \\ \partial_t (\alpha_k E_k) + \partial_x (\alpha_k U_k (E_k + P_k)) + P^i \partial_t (\alpha_k) = T_k V^i \end{cases} \quad (\text{C.7})$$

Approximations at the end of the evolution process will be noted \tilde{Z} . Obviously, even if the local pressures are in equilibrium in all cells *at the beginning of the time step* (that is: $(P_1)_i^n = (P_2)_i^n$), this will no longer hold at the end of the time step, which means that $\tilde{P}_1 \neq \tilde{P}_2$.

The pressure-relaxation step will then correct the prediction in each cell, by computing approximations of the solution of the following set of ODE:

$$\begin{cases} \partial_t (\alpha_1) = \lambda(P_1 - P_2) \\ \partial_t (m_k) = 0 \\ \partial_t (m_k U_k) = 0 \\ \partial_t (\alpha_k E_k) + P^i \partial_t (\alpha_k) = 0 \end{cases} \quad (\text{C.8})$$

Actually, both m_k and U_k remain unchanged during this process. In practice we shall set:

$$\lambda = \alpha_1 \alpha_2 \theta^{-1} / (P_1 + P_2) \quad (\text{C.9})$$

Hence, this in practice will update values of (α_1, P_1, P_2) .

Now, two frames should be distinguished. In the first one, where one aims at computing true approximations of the two-fluid two-pressure model, the relaxation time θ associated with λ should remain non zero. On the contrary, the standard two-fluid model requires instantaneous relaxation process ($\lambda = +\infty$). The final time approximation is noted in any case Z^{n+1} .

We will focus herein on the computation of the standard two-fluid model, and thus will detail properties pertaining to the latter systems (C.7)-(C.8) in the continuous and discrete frameworks. The reader is referred to [34] for details on the numerical procedures to cope with the relaxation process when λ is finite.

C.3 Comments on both steps

C.3.1 Properties of the two-pressure model

We very briefly recall herein some important properties of the two-fluid two-pressure model *when the closures (C.5)-(C.6) hold*:

$$\begin{cases} \partial_t (\alpha_1) + V^i \partial_x (\alpha_1) = \lambda(P_1 - P_2) \\ \partial_t (m_k) + \partial_x (m_k U_k) = 0 \\ \partial_t (m_k U_k) + \partial_x (m_k U_k^2 + \alpha_k P_k) - P^i \partial_x (\alpha_k) = T_k \\ \partial_t (\alpha_k E_k) + \partial_x (\alpha_k U_k (E_k + P_k)) + P^i \partial_t (\alpha_k) = T_k V^i \end{cases} \quad (\text{C.10})$$

The system (C.10) is hyperbolic. Unless some resonance occurs, the set of eigenvectors spans \mathbb{R}^7 . If we note $\rho_k c_k^2 = \gamma_k P_k$, eigenvalues are real:

$$\begin{cases} \lambda_1 = V_i \\ \lambda_2 = U_1 - c_1, \quad \lambda_3 = U_1, \quad \lambda_4 = U_1 + c_1 \\ \lambda_5 = U_2 - c_2, \quad \lambda_6 = U_2, \quad \lambda_7 = U_2 + c_2 \end{cases} \quad (\text{C.11})$$

Fields 2,4,5,7 are genuinely non linear and the fields 1,3,6 are linearly degenerated (owing to (C.5)). Regular solutions of the latter system are such that α_k remain positive, assuming admissible inlet boundary conditions, and regular velocity fields. In addition, under the same assumptions, m_1 and m_2 remain positive. A similar property holds for P_k , for perfect gas laws and assuming that $\mu(1 - \mu) = 0$.

We need to introduce specific entropies s_k in agreement with :

$$\gamma_k P_k \partial_{P_k} (s_k) + \rho_k \partial_{\rho_k} (s_k) = 0 \quad (\text{C.12})$$

where:

$$\rho_k (c_k)^2 = (\partial_{P_k} (e_k))^{-1} \left(\frac{P_k}{\rho_k} - \rho_k \partial_{\rho_k} (e_k) \right) \quad (\text{C.13})$$

A crucial point to note is that the following inequality holds for regular solutions:

$$\partial_t (\eta) + \partial_x (F_\eta) \leq 0 \quad (\text{C.14})$$

introducing:

$$\eta = -m_1 \text{Ln}(s_1) - m_2 \text{Ln}(s_2) \quad (\text{C.15})$$

and:

$$F_\eta = -m_1 \text{Ln}(s_1) U_1 - m_2 \text{Ln}(s_2) U_2 \quad (\text{C.16})$$

This is a keystone for the whole procedure.

C.3.2 Properties of the relaxation step

We consider here the pressure relaxation step, that is:

$$\begin{cases} \partial_t (\alpha_1) = \lambda(P_1 - P_2) \\ \partial_t (m_k) = 0 \\ \partial_t (m_k U_k) = 0 \\ \partial_t (\alpha_k E_k) - (-1)^k P^i \partial_t (\alpha_1) = 0 \end{cases} \quad (\text{C.17})$$

with an initial condition in the admissible range ($P_k > 0, \alpha_k > 0$).

Throughout the pressure relaxation step, we note that:

$$m_k \partial_t (e_k) = -P^i \partial_t (\alpha_k) \quad (\text{C.18})$$

and:

$$\alpha_k \partial_t (\rho_k) = -\rho_k \partial_t (\alpha_k) \quad (\text{C.19})$$

Thus, we get:

$$\partial_t (s_k) = (\partial_{P_k} (e_k))^{-1} \partial_{P_k} (s_k) (\partial_t (e_k) - \frac{P_k}{(\rho_k)^2} \partial_t (\rho_k)) \quad (\text{C.20})$$

or:

$$\partial_t (s_k) = (\partial_{P_k} (e_k))^{-1} \partial_{P_k} (s_k) \left(\frac{P_k - P^i}{m_k} \right) \partial_t (\alpha_k) \quad (\text{C.21})$$

Hence:

$$\frac{m_k}{s_k} \partial_t (s_k) = a_k (P_k - P^i) \partial_t (\alpha_k) \quad (\text{C.22})$$

Since:

$$\partial_t (\eta) = - \sum_{k=1}^2 \frac{m_k}{s_k} \partial_t (s_k) \quad (\text{C.23})$$

we get :

$$\partial_t (\eta) = - \frac{a_1 a_2}{(1 - \mu) a_1 + \mu a_2} (P_1 - P_2) \partial_t (\alpha_1) \quad (\text{C.24})$$

Thus :

$$\partial_t (\eta) = - \frac{a_1 a_2}{(1 - \mu) a_1 + \mu a_2} \lambda (P_1 - P_2)^2 \quad (\text{C.25})$$

We may get some description of the minimum value obtained in M_0 :

$$\partial_t (\eta) = 0 \quad \Leftrightarrow \quad P_2 - P_1 = 0 \quad (\text{C.26})$$

Even more, the second derivative around M_0 is:

$$\partial_{t^2} ({}^2\eta) |_{M_0} = \frac{a_1 a_2}{(1 - \mu) a_1 + \mu a_2} \left(\frac{\gamma_1 P_1}{\alpha_1} + \frac{\gamma_2 P_2}{\alpha_2} \right) X^2 \quad (\text{C.27})$$

setting $X = \partial_t (\alpha_1)$, and using the identity:

$$\partial_t (P_k) = (\partial_{P_k} (e_k))^{-1} (\partial_t (e_k) - (\partial_{\rho_k} (e_k)) \partial_t (\rho_k)) \quad (\text{C.28})$$

Since $\gamma_k P_k = \rho_k (c_k)^2$ is positive, $\partial_{t^2} (\eta)_{M_0}$ is thus positive. This ensures that the instantaneous relaxation of pressure minimizes the entropy of the whole system. This result holds true for any EOS.

C.4 Schemes and main properties

C.4.1 A consistant relaxation method

We only discuss herein the relaxation step when restricting to instantaneous relaxation. We need to introduce a notion of "consistency condition on pressure" as follows. If we assume a perfect balance on initial values of pressures:

$$\tilde{P}_1 = \tilde{P}_2 = \phi \quad (\text{C.29})$$

this should imply that:

$$P^{n+1} = \phi \quad (\text{C.30})$$

and therefore: $\alpha_k^{n+1} = \tilde{\alpha}_k$. In other words, the relaxation step must be a "ghost step" in that particular case. We thus focus on the following scheme, which is exactly the one used in [23]:

$$\begin{cases} (P_k)_i^{n+1} = (P)_i^{n+1} \\ (m_k)_i^{n+1} = (\tilde{m}_k)_i \\ (m_k U_k)_i^{n+1} = (\tilde{m}_k)_i (\tilde{U}_k)_i \\ (\alpha_k E_k)_i^{n+1} - (\tilde{\alpha}_k)_i (\tilde{E}_k)_i + (P)_i^{n+1} ((\alpha_k)_i^{n+1} - (\tilde{\alpha}_k)_i) = 0 \end{cases} \quad (\text{C.31})$$

The latter equation is equivalent to:

$$(m_k e_k)_i^{n+1} - (\tilde{m}_k)_i (\tilde{e}_k)_i + (P)_i^{n+1} ((\alpha_k)_i^{n+1} - (\tilde{\alpha}_k)_i) = 0 \quad (\text{C.32})$$

owing to the first three mesh schemes.

If we moreover restrict to perfect gas EOS within each step, setting thus: $(\gamma_k - 1)\rho_k e_k = P_k$, in agreement with condition $\gamma_k > 1$, we immediatly get:

$$\frac{(\alpha_k P_k)_i^{n+1} - (\tilde{\alpha}_k \tilde{P}_k)_i}{\gamma_k - 1} + (P)_i^{n+1} ((\alpha_k)_i^{n+1} - (\tilde{\alpha}_k)_i) = 0 \quad (\text{C.33})$$

We deduce:

$$P_i^{n+1} = \frac{\tilde{\alpha}_{1i}\gamma_2(\tilde{P}_1)_i + \tilde{\alpha}_{2i}\gamma_1(\tilde{P}_2)_i}{\tilde{\alpha}_{1i}\gamma_2 + \tilde{\alpha}_{2i}\gamma_1} \quad (\text{C.34})$$

and subsequently $(P_k)_i^{n+1} = P_i^{n+1}$ (for $k = 1, 2$), but also:

$$(\alpha_k)_i^{n+1} = (\tilde{\alpha}_k)_i \left(\frac{\gamma_k - 1}{\gamma_k} + \frac{(\tilde{P}_k)_i}{\gamma_k P_i^{n+1}} \right) \quad (\text{C.35})$$

Property 1: Both P_i^{n+1} and $(\alpha_1)_i^{n+1}(1 - \alpha_1)_i^{n+1}$ remain positive through the relaxation step, assuming relevant initial data.

C.4.2 Basic schemes used to compute the evolution step

The numerical method used to compute approximate solutions of the convection step is exactly the one described in [34]. It is thus not recalled in this paper. It is a Finite volume method, where the numerical convective fluxes at each cell interface rely either on Rusanov scheme, the exact Godunov scheme or on the approximate Godunov scheme VFRoe-ncv (see [31]). The time step is chosen to

agree with the standard CFL condition: $CFL = 0.5$.

Property 2:

2.1- The Rusanov scheme enables to maintain positive values of the void fraction and partial masses, assuming standard CFL condition.

2.2- The exact Godunov scheme preserves the positivity of expected positive components.

Obviously, if one aims at computing the standard two-fluid model, one needs to initialize first the "mean pressure" $(P)_i^0$, and then to define the cell phasic pressures as follows: $(P_1)_i^0 = (P)_i^0$ and $(P_2)_i^0 = (P)_i^0$, for any cell with subscript i . The whole procedure will then ensure that a pressure equilibrium is achieved at the end of each time step, owing to the relaxation procedure.

C.5 Numerical results

We note that we use afterwards the Baer-Nunziato closure, which means that $\mu = 0$, which turns to $V_i = U_2$, and $P^i = P_1$.

C.5.1 The Riemann problem

We consider initial conditions issuing from [23]. Thus, we start the computation with :

$$\begin{aligned} U_1(x,t=0) &= U_2(x,t=0) = 0 \\ \alpha_1(x,t=0) &= 0.25 & P(x,t=0) &= 2.10^7 \\ h_1(x,t=0) &= 3.09310^6 & h_2(x,t=0) &= 1.3510^6 \end{aligned}$$

for $x < 0.5$, and :

$$\begin{aligned} U_1(x,t=0) &= U_2(x,t=0) = 0 \\ \alpha_1(x,t=0) &= 0.25 & P(x,t=0) &= 1.510^7 \\ h_1(x,t=0) &= 3.09310^6 & h_2(x,t=0) &= 2.3510^6 \end{aligned}$$

for $x > 0.5$. A coarse mesh contains 50 cells, a medium mesh contains 1000 cells, and the finer mesh contains 250000 cells. The straight line corresponds to the computation where drag effects have been omitted, squares denote approximations where the drag coefficient is computed with a bubble particle mean diameter $d = 1.10^{-3}$, and circles represent solutions for $d = 1.10^{-6}$.

For each computation, we plot the modulus of non zero imaginary part of eigenvalues, if meaningful. The physical time for simulation is the same in each case.

C.5.2 Omitting drag effects

Figures C.1 , C.2, C.3 and C.4 show the void fraction, the mean pressure and velocities. Figure C.5 shows that some complex eigenvalues arise in the computation, which are obviously correlated with the relative velocity U_r , but the coarse mesh with 50 cells provides a smooth solution. The solution nonetheless shows a strange behaviour on the void fraction, mean pressure, velocity and the relative velocity $U_2 - U_1$ profiles when using a mesh with 1000 cells (see figures C.6 , C.7, C.8, C.9, C.10). The solution explodes when using a mesh with 5000 cells.

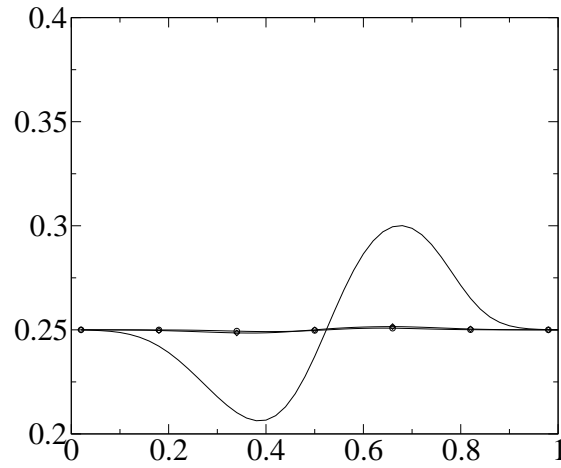


FIG. C.1 – *Riemann problem 1: void fraction. Straight line (no drag), squares ($d = 1.10^{-3}$), circles($d = 1.10^{-6}$) - 50 cells*

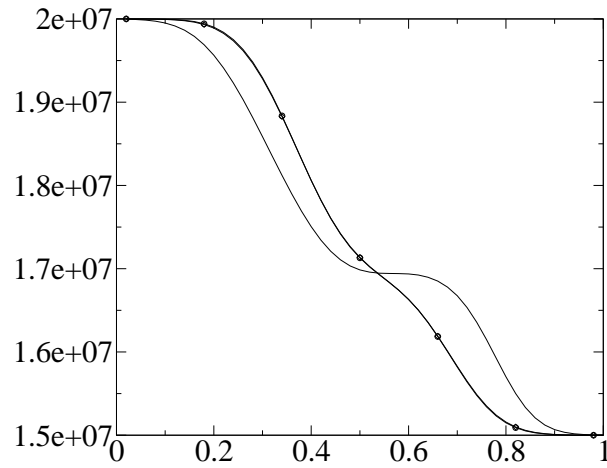


FIG. C.2 – *Riemann problem 1: mean pressure P . Straight line (no drag), squares ($d = 1.10^{-3}$), circles($d = 1.10^{-6}$) - 50 cells*

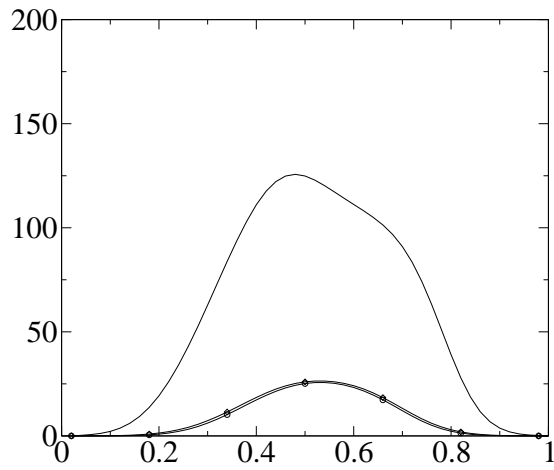


FIG. C.3 – Riemann problem 1: velocity U_1 . Straight line (no drag), squares ($d = 1.10^{-3}$), circles($d = 1.10^{-6}$) - 50 cells

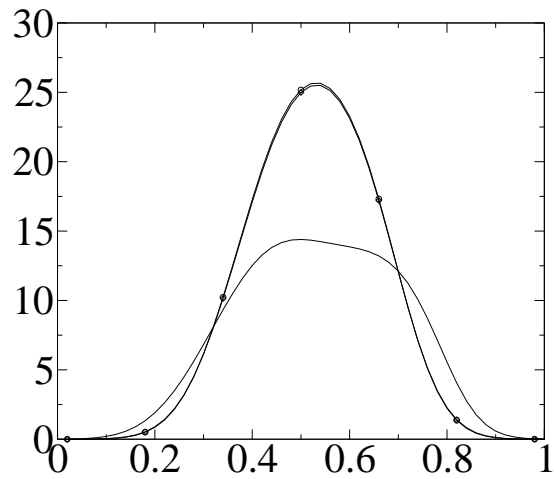


FIG. C.4 – Riemann problem 1: velocity U_2 . Straight line (no drag), squares ($d = 1.10^{-3}$), circles($d = 1.10^{-6}$) - 50 cells

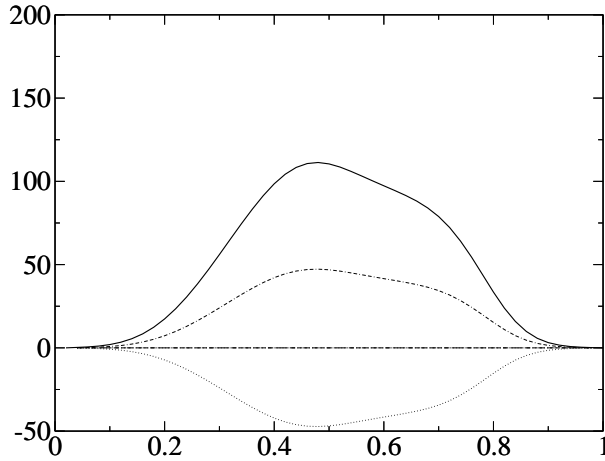


FIG. C.5 – *Riemann problem 1: velocity U_r and imaginary part of eigenvalues. (no drag) - 50 cells*

C.5.3 Accounting for drag effects

When accounting for drag effects, the order of magnitude of the relative velocity is clearly reduced. Focusing on the mesh with 1000 cells, it occurs that the pressure profile is much smoother (see figures C.7). This holds true for velocities too.

Nonetheless, we note that the imaginary part of eigenvalues is non zero when $d = 10^{-3}$ (see figure C.10). If one turns then to the same particle size on a much finer mesh with 250000 cells, it clearly arises that the void fraction is once again much polluted around the location $x = 0.52$ (see figure C.11). An amazing point is that the pressure profile still seems to be regular around this location on this particular mesh (see figure C.12). Velocities are plotted on figures C.13 and C.14. Figure C.16 displays the correlation between the void fraction and the relative velocity around $x = 0.52$.

Actually, one retrieves a blow up of the code on a mesh with 10^6 cells.

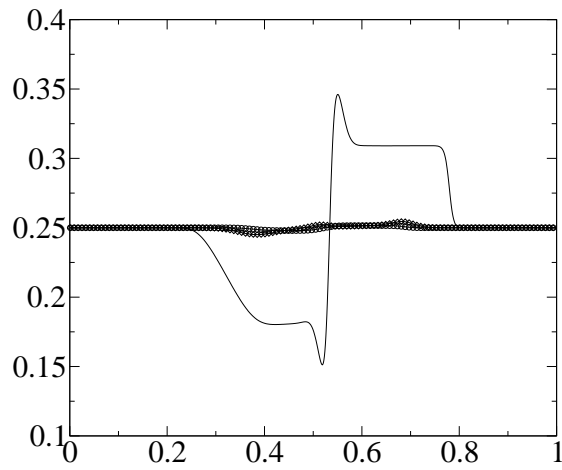


FIG. C.6 – Riemann problem 1: void fraction. Straight line (no drag), squares ($d = 1.10^{-3}$), circles ($d = 1.10^{-6}$) - 1000 cells

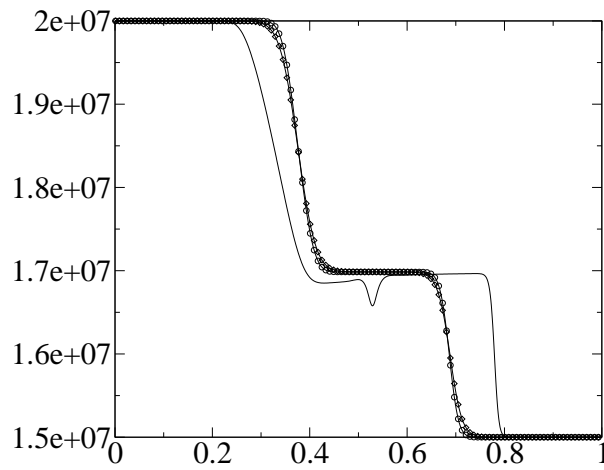


FIG. C.7 – Riemann problem 1: mean pressure P . Straight line (no drag), squares ($d = 1.10^{-3}$), circles ($d = 1.10^{-6}$) - 1000 cells

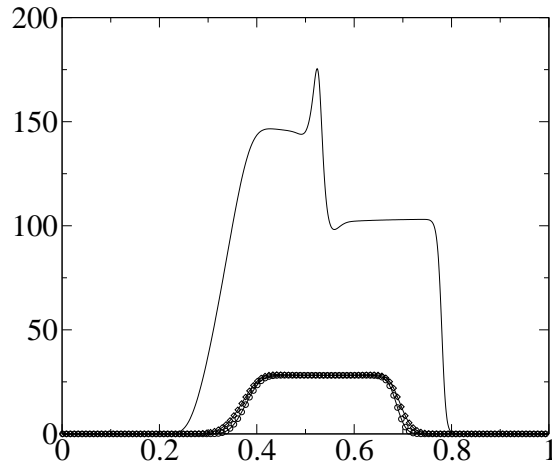


FIG. C.8 – *Riemann problem 1: velocity U_1 . Straight line (no drag), squares ($d = 1.10^{-3}$), circles($d = 1.10^{-6}$) - 1000 cells*

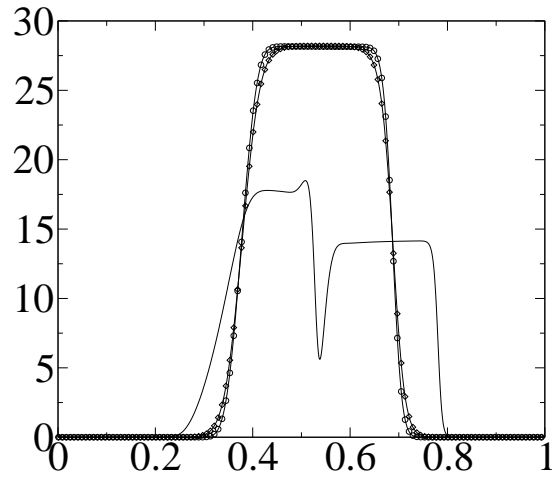


FIG. C.9 – *Riemann problem 1: velocity U_2 . Straight line (no drag), squares ($d = 1.10^{-3}$), circles($d = 1.10^{-6}$) - 1000 cells*

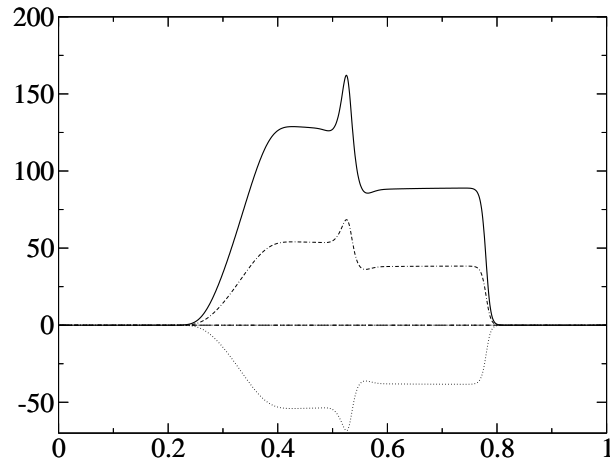


FIG. C.10 – *Riemann problem 1: velocity U_r and imaginary part of eigenvalues. (no drag) - 1000 cells*

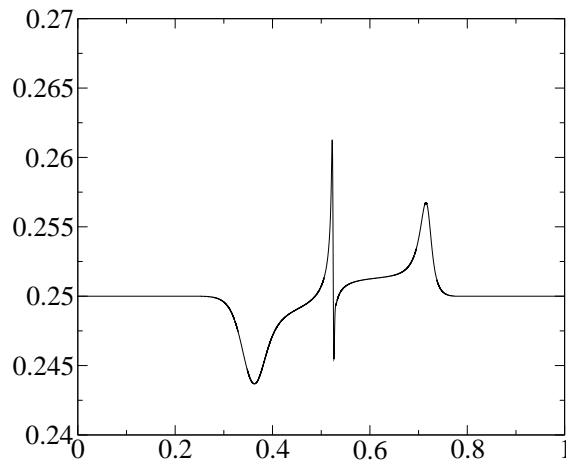
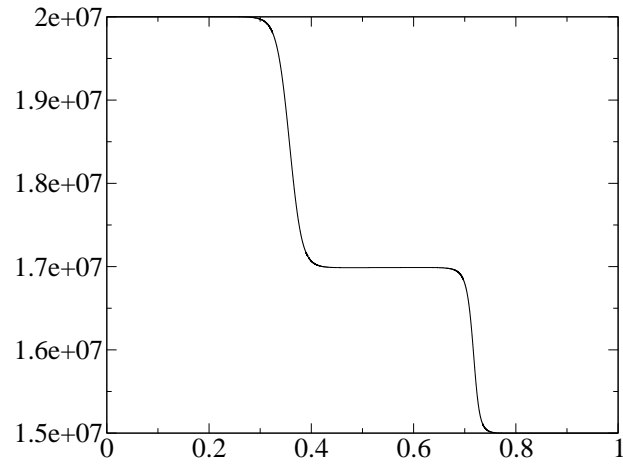
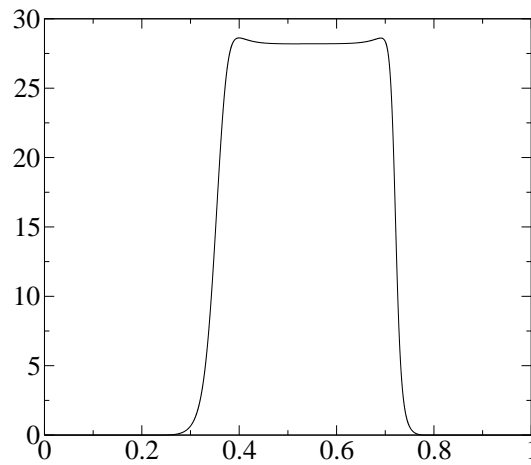


FIG. C.11 – *Riemann problem 1: void fraction. ($d = 1.10^{-3}$) - 250000 cells*

FIG. C.12 – Riemann problem 1: mean pressure. ($d = 1.10^{-3}$) - 250000 cellsFIG. C.13 – Riemann problem 1: U_1 . ($d = 1.10^{-3}$) - 250000 cells

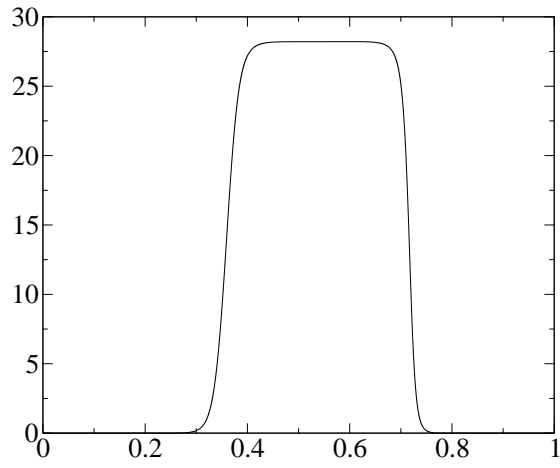


FIG. C.14 – *Riemann problem 1: U_2 . ($d = 1.10^{-3}$) - 250000 cells*

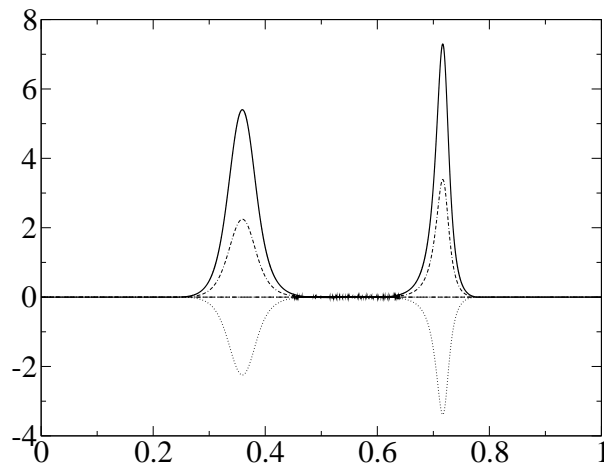


FIG. C.15 – *Riemann problem 1: relative velocity U_r and imaginary part of eigenvalues. ($d = 1.10^{-3}$) - 250000 cells*

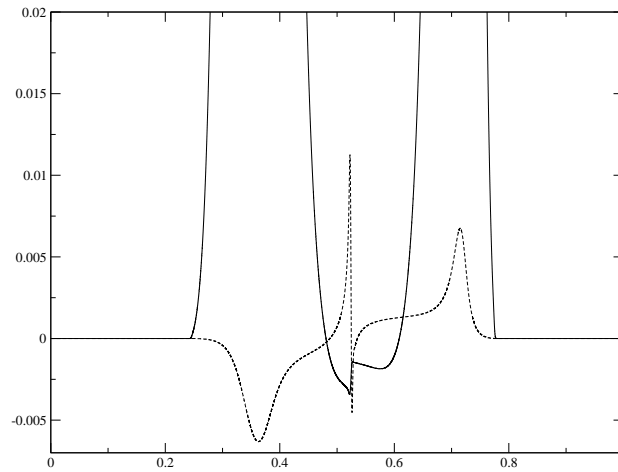


FIG. C.16 – Riemann problem 1: zooming the relative velocity U_r and the void fraction. ($d = 1.10^{-3}$)
- 250000 cells

C.6 Conclusion

We have a twofold conclusion:

(i) The numerical method which has been proposed herein, which combines the use of the two-fluid two-pressure approach and the relaxation procedure, enables to cope with both the two-fluid two-pressure model and the standard two-fluid model, without specific restriction on the time stepping;

(ii) The overall algorithm is stable, and fortunately does not hide potential deficiencies of continuous models regarding hyperbolicity.

It may thus be seen as a possible tool to compute both well-posed initial-value problems on any mesh, and possibly locally ill-posed models on "coarse meshes".

C.7 Acknowledgements

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Annexe D

Complete set of numerical results
obtained for the chapter 4

D.1 Basic test cases without source term

D.1.1 A contact wave traveling from HEM to HRM($\Gamma = 0$)

We are in the first configuration (fig. (4.2)). The results show the computed solutions when the contact wave has passed through the coupling interface $x = 0$. The dashed lines represent the initial data and the plain line stands for the solution computed by our numerical scheme.

a) The initial data for the HRM($\Gamma = 0$) model is in equilibrium:

domain :	HEM	HEM	HRM($\Gamma = 0$)
U	10	10	10
P	150e5	150e5	150e5
ρ	1000	900	900
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_R, \rho_R)$	$C_{eq}(P_R, \rho_R)$

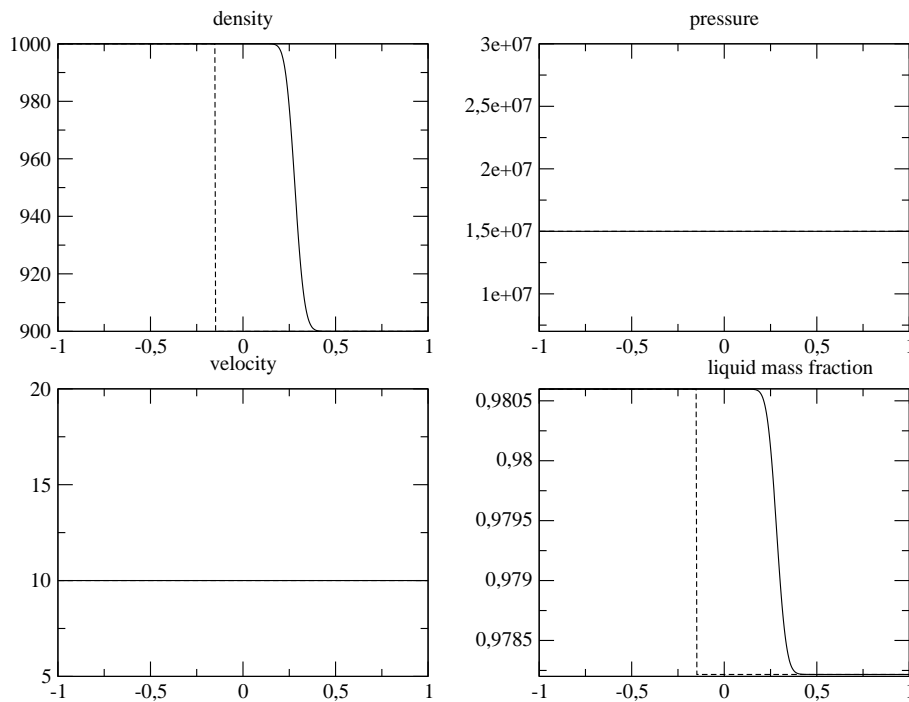


FIG. D.1 – The initial discontinuity is located at $x = -0.15$. Preservation of the discrete contact solution through the coupling interface $x = 0$. The HRM model is in equilibrium. We thus check the above mentioned result in the preceding section.

b)The initial data for the HRM($\Gamma = 0$) model is not in equilibrium:

	HEM	HEM	HRM($\Gamma = 0$)
U	10	10	10
P	150e5	150e5	150e5
ρ	1000	900	900
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_R, \rho_R)$	0.978

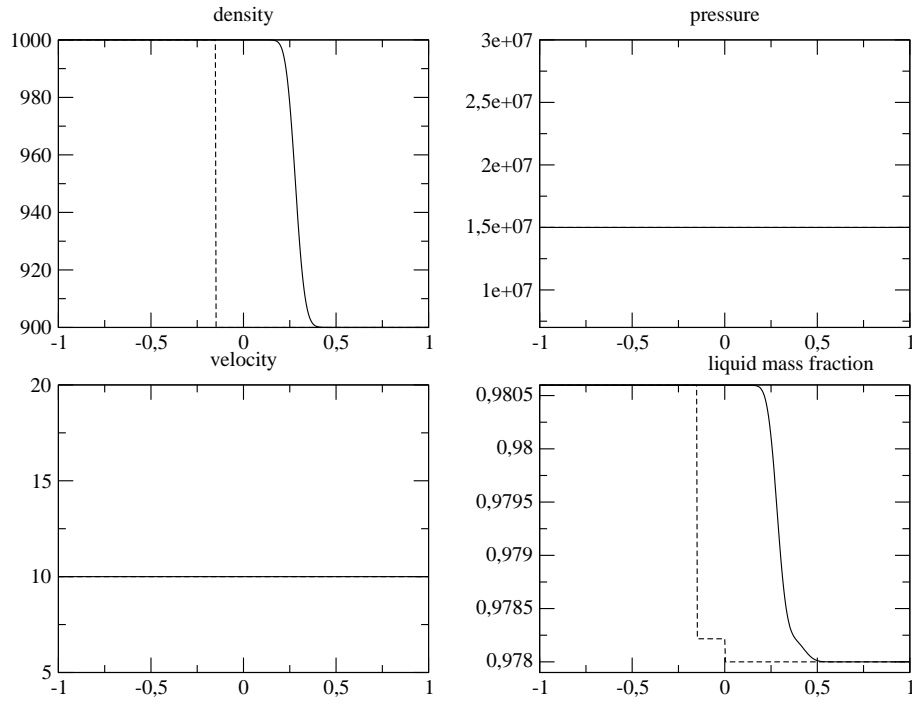


FIG. D.2 – The initial discontinuity is located at $x = -0.15$. Preservation of the discrete contact solution through the coupling interface $x = 0$. The HRM model is not in equilibrium. We thus check the above mentioned result in the preceding section.

D.1.2 A contact wave traveling from HRM($\Gamma = 0$) to HEM

We are in the first configuration (fig. (4.3)). The results show the computed solutions when the contact wave has passed through the coupling interface $x = 0$. The dashed lines represent the initial data and the plain line stands for the solution computed by our numerical scheme.

a) The initial data for the HRM($\Gamma = 0$) model is in equilibrium:

domain :	HEM	HRM($\Gamma = 0$)	HRM($\Gamma = 0$)
U	-10	-10	-10
P	150e5	150e5	150e5
ρ	900	900	1000
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_R, \rho_R)$

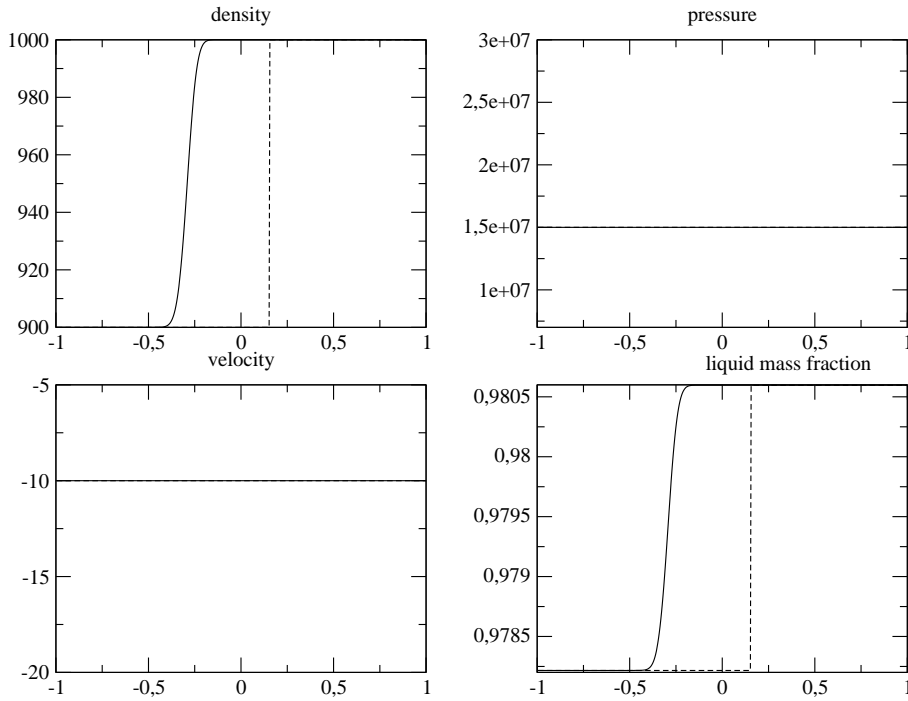


FIG. D.3 – The initial discontinuity is located at $x = 0.15$. Preservation of the discrete contact solution through the coupling interface $x = 0$. The HRM model is in equilibrium. We thus check the above mentioned result in the preceding section.

b) The initial data for the HRM($\Gamma = 0$) model is not in equilibrium:

domain :	HEM	HRM($\Gamma = 0$)	HRM($\Gamma = 0$)
U	-10	-10	-10
P	150e5	150e5	150e5
ρ	990	990	1000
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_L, \rho_L)$	0.9805

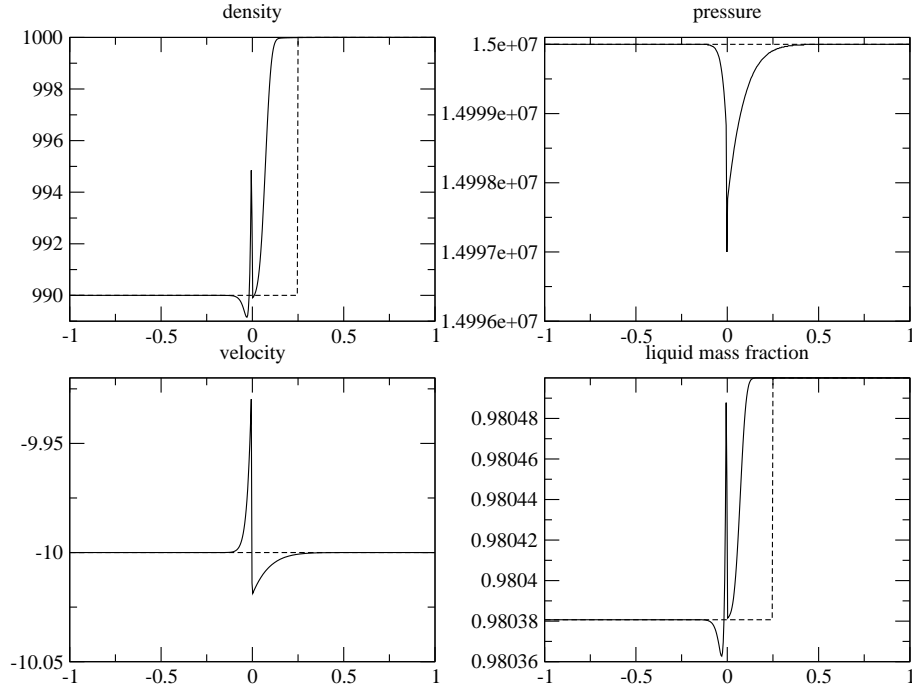


FIG. D.4 – The initial discontinuity is located at $x = 0.25$. The HRM model is not in equilibrium. We thus check the above mentioned result in the preceding section. The contact wave is not preserved.

We check that the contact wave is not preserved, due to the fact that $C_{eq}(P_L, \rho_L) \neq 0.9805$ together with $U_0 < 0$.

The numerical fluxes at cell interfaces are plotted on figure (D.5). The cell fluxes computed on the basis of the cell values are plotted on the figure (D.6). We can check that no pollution arises on the interface $x = 0$ (or equivalently $n = 250$) for the numerical fluxes computed with the approximate Godunov scheme and that there is only a small glitch on the cell flux profiles in the first cell on the left side of $x = 0$.

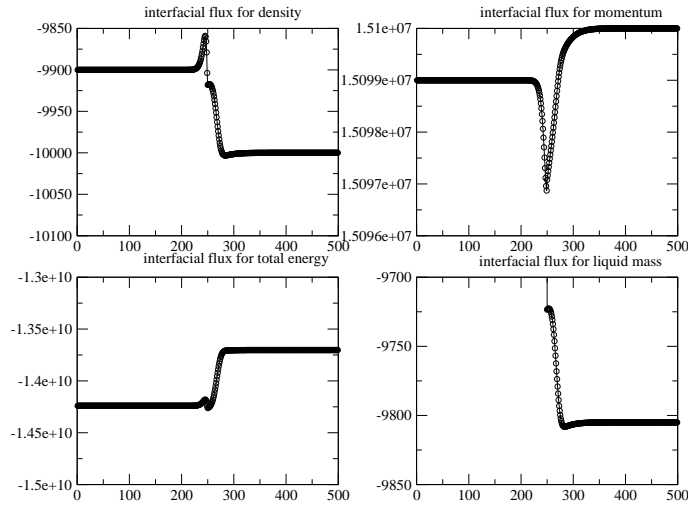


FIG. D.5 – This figure shows the interfacial fluxes computed with our numerical schemes. The x -axis represent the number of the interfaces between cells including boundary interfaces. The coupling interface has the number 250. We insist that there is no relevant data available for the liquid mass fraction in the HEM domain.

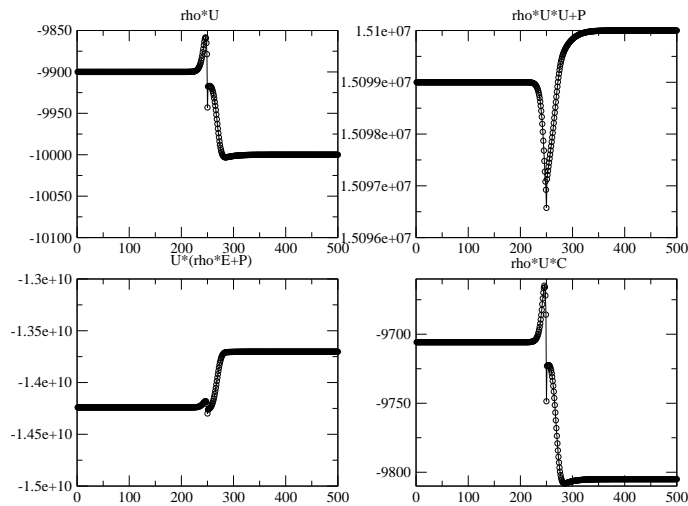


FIG. D.6 – This figure shows the analytical fluxes computed using the cell values.

D.2 Test cases with the full HRM model

We consider again the preceding test cases but we now include the source term in the HRM domain. Of course, if $C = C_{eq}$ in the HRM domain, we get: $\Gamma = 0$; thus the results should be the same as in the preceding section.

D.2.1 A "contact wave" traveling from HEM to HRM

Once again we focus on the first configuration (fig. (4.2)). We plot computational results when the contact when has passed the coupling interface $x = 0$. The dashed lines still represent the initial data and the plain lines show the computational cell values.

a) HRM at equilibrium:

domain :	HEM	HEM	HRM
U	10	10	10
P	150e5	150e5	150e5
ρ	1000	900	900
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_R, \rho_R)$	$C_{eq}(P_R, \rho_R)$

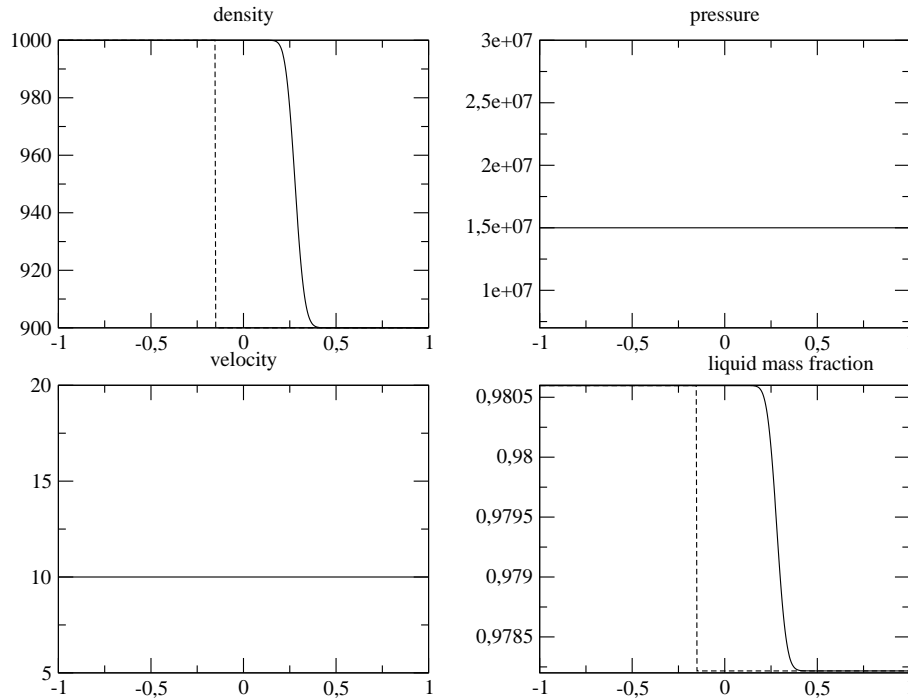


FIG. D.7 – The initial discontinuity lies at $x = -0.15$. As expected, the discrete contact solution is preserved. The pressure and the velocity remain uniform and constant.

b) HRM out of equilibrium:

We present here two test cases. In the first one (figure (D.8)) a contact travels from the HEM domain to the HRM domain. The discontinuity of the liquid mass fraction at the coupling interface $x = 0$ due to the disequilibrium of the HRM model generates a pollution. This pollution has the same magnitude of order than the discontinuity of the contact wave. In the second test case (figure (D.9)) we focus on this pollution.

	HEM	HEM	HRM
U	10	10	10
P	150e5	150e5	150e5
ρ	1000	900	900
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_R, \rho_R)$	0.9782

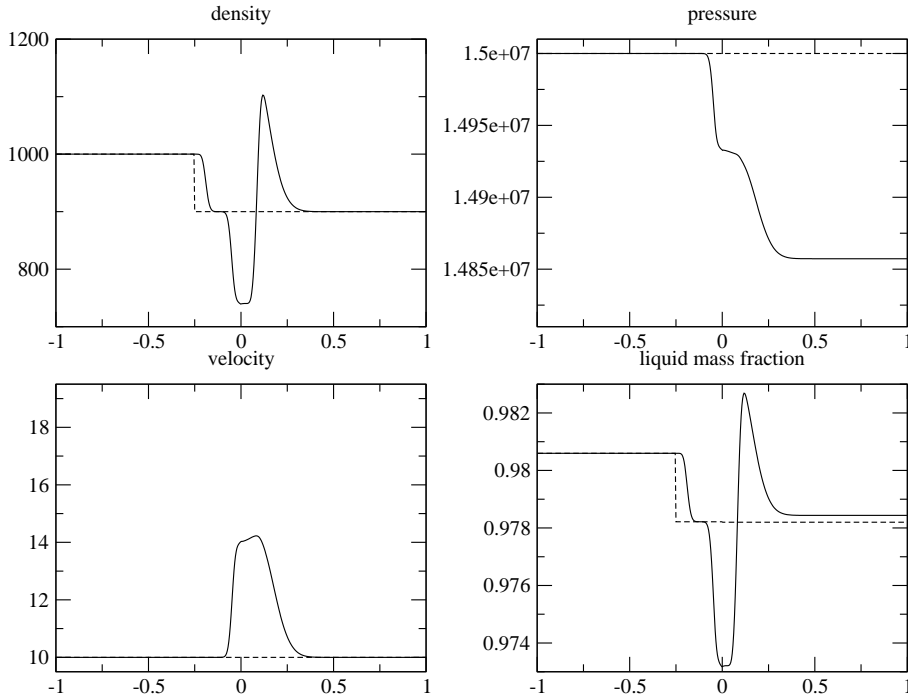


FIG. D.8 – *The initial discontinuity is located at $x = -0.25$. The contact wave has not reached $x = 0$. The discrete contact solution is not preserved. The pollution at the coupling interface appears immediately.*

On the basis of the set of equations (4.30) we get:

$$\begin{cases} \partial_t (C) = \Gamma \\ \partial_t (P) = -(\partial_P (e_{HRM}))^{-1} \partial_C (e_{HRM}) \Gamma \end{cases} \quad (\text{D.1})$$

The initial conditions provide $\Gamma > 0$, and thus $\partial_t (C)|_{t=0} > 0$ and $\partial_t (P)|_{t=0} < 0$ which clearly appears on the right of the profiles. This relaxation process generates the pollution located at the coupling interface. The discrete contact solution is not preserved.

	HEM	HEM	HRM
U	10	10	10
P	150e5	150e5	150e5
ρ	900	900	900
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_R, \rho_R)$	0.9782

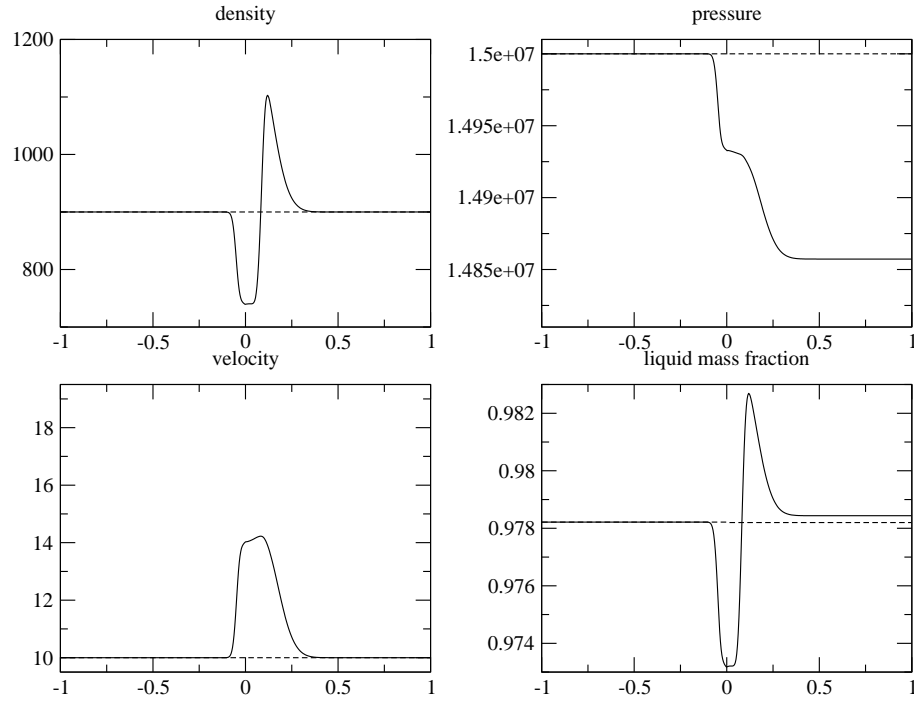


FIG. D.9 – The initial discontinuity is located at $x = -0.25$. The pollution at the coupling interface is due to the disequilibrium of the liquid mass fraction and the relaxation process.

D.2.2 A "contact wave traveling" from HRM to HEM

This is the counterpart of the figure (D.7), but the contact wave is now initiated in the HRM domain and travels to the left.

a) HRM at equilibrium:

domain :	HEM	HRM	HRM
U	-10	-10	-10
P	150e5	150e5	150e5
ρ	900	900	1000
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_R, \rho_R)$

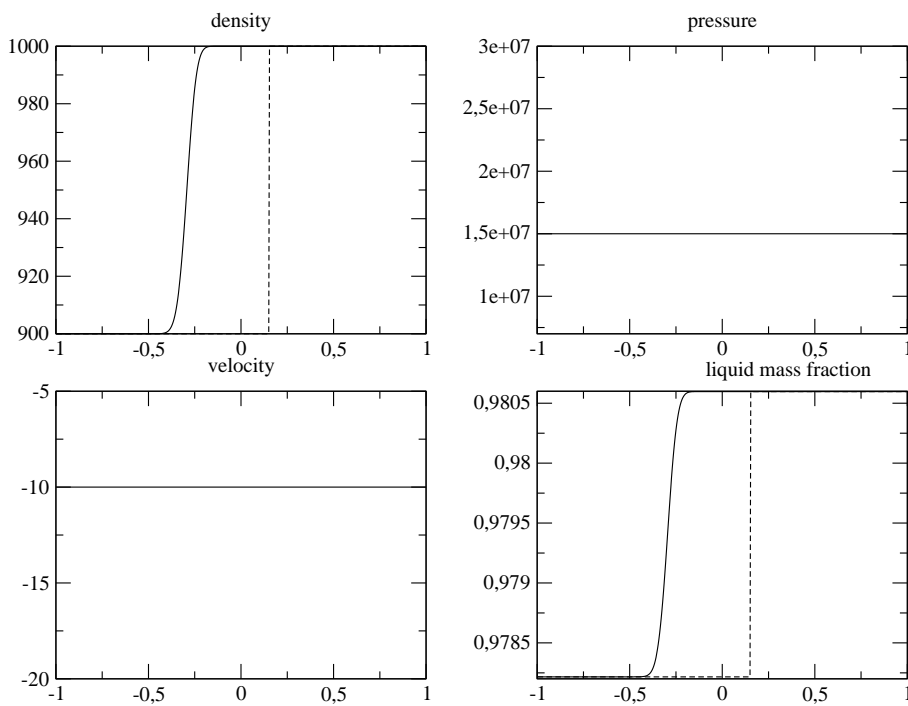


FIG. D.10 – The initial discontinuity is located at $x = 0.15$. As expected, no trouble arises in the vicinity of the coupling interface between the HEM and HRM models.

b) HRM out of equilibrium:

Though initialized with uniform pressure and velocity profiles, the contact wave is no longer a solution, due to the occurrence of the source term Γ in the HRM domain. Two genuinely non-linear waves developed in the numerical solution. The contact discontinuity initially travels to the left but due to the increase of the velocity it finally travels to the right. At the current time $t = 0.03$, the segment approximatively delimited by $x = 0.56$ and $x = 0.6$ does not contain vapor, $C = 1.0$.

domain :	HEM	HRM	HRM
U	-10	-10	-10
P	150e5	150e5	150e5
ρ	990	990	1000
C	$C_{eq}(P_L, \rho_L)$	$C_{eq}(P_L, \rho_L)$	0.9805

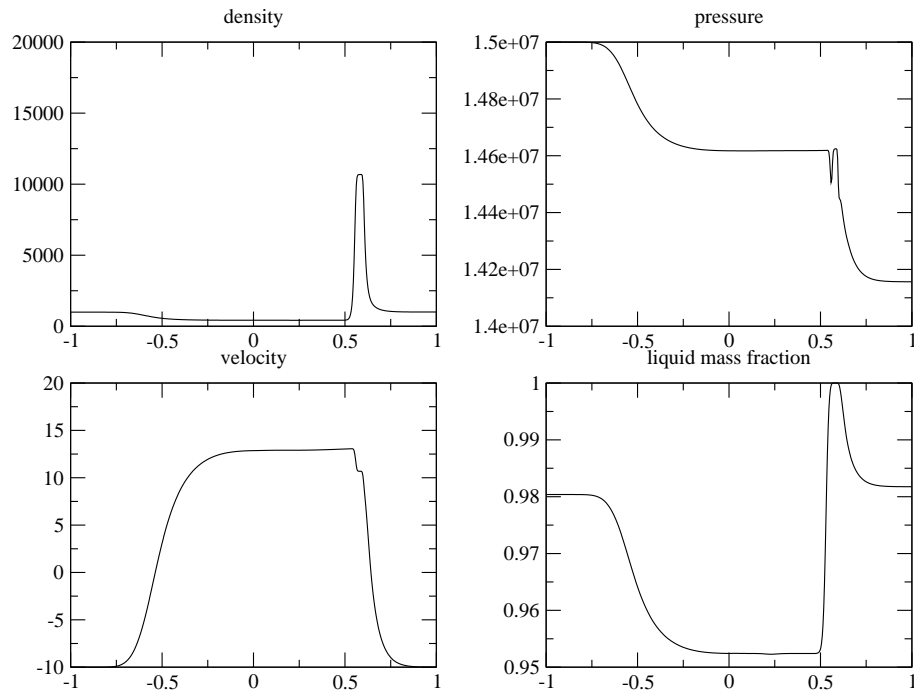


FIG. D.11 – The initial discontinuity is located at $x = 0.25$.

D.3 Riemann problems test cases

Results are plotted at time $t = 0.025$. Initial discontinuity is located at $x = \pm 0.25$. The following test cases are Riemann problems with a discontinuity of the initial data located at $x = -0.25$ (when focusing on a wave travelling from the HEM model to the HRM model) or at $x = +0.25$ (when focusing on a wave travelling from the HRM model to the HEM model). The initial data are such that the HRM model is initially in an equilibrium state (i.e. $C = C_{eq}$ in all the computational domain). In each case we have plotted the results before the contact discontinuity wave (corresponding to the LD field(s)) hits the coupling interface. Only one wave thus has crossed this interface.

Two different constant time scale are used. For the smaller one $\tau_0^2 = 10^{-3}$ the solutions computed for the HRM model are close to the solutions computed for the HEM model. But for $\tau_0^1 = 1$, the two models provides very different solutions. The intermediate states and waves speed are very different.

D.3.1 A shock wave traveling from HEM domain to HRM domain

domain :	HEM	HEM	HRM
U	0	0	0
P	160e5	158e5	158e5
ρ	1000	990	990
C	none	none	0.979261526
C_{eq}	0.979212418	0.979261526	0.979261526

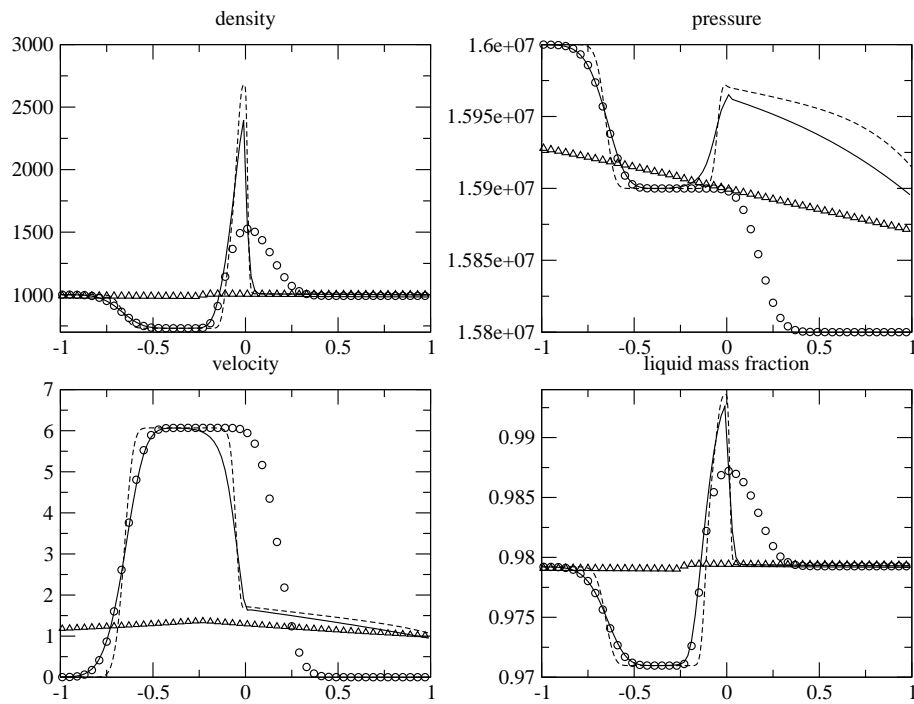


FIG. D.12 – Constant time scale τ_0^1 . The initial discontinuity is in the HEM domain. A shock wave travels to the right and goes through the coupling interface ($x = 0$). A rarefaction wave travels to the left. A contact discontinuity travels to the right but is still on the left of the coupling interface. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, There are no results for HEM/HRM 500 cells and 10000 cells because the computed solution goes out from D_{HRM} .

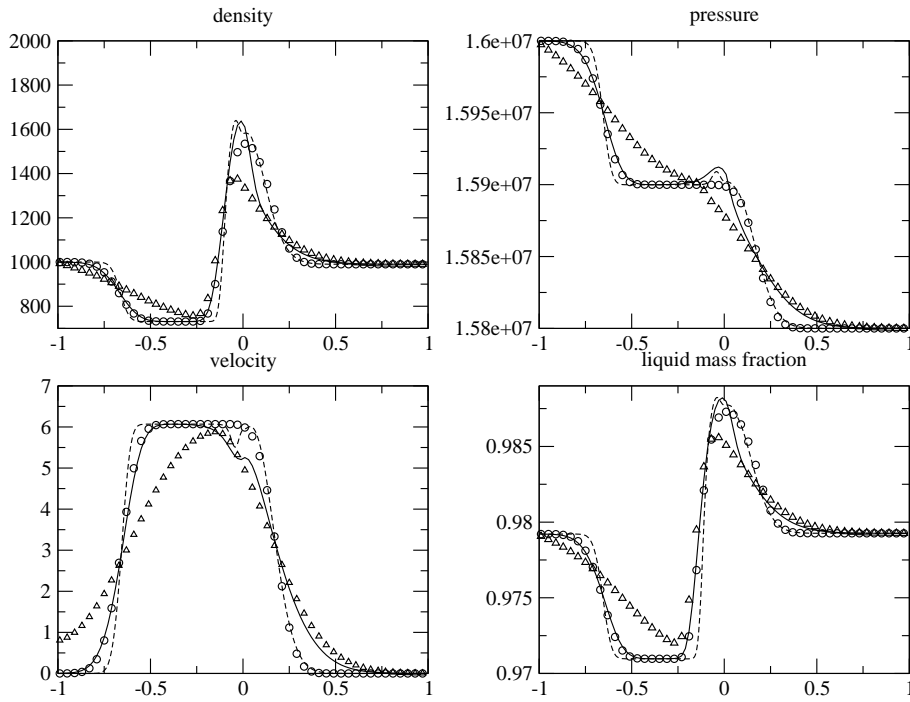


FIG. D.13 – Constant time scale τ_0^2 . The initial discontinuity is in the HEM domain. A shock wave travels to the right and goes through the coupling interface ($x = 0$). A rarefaction wave travels to the left. A contact discontinuity travels to the right but is still on the left of the coupling interface. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, dashed line=HEM/HRM 500 cells.

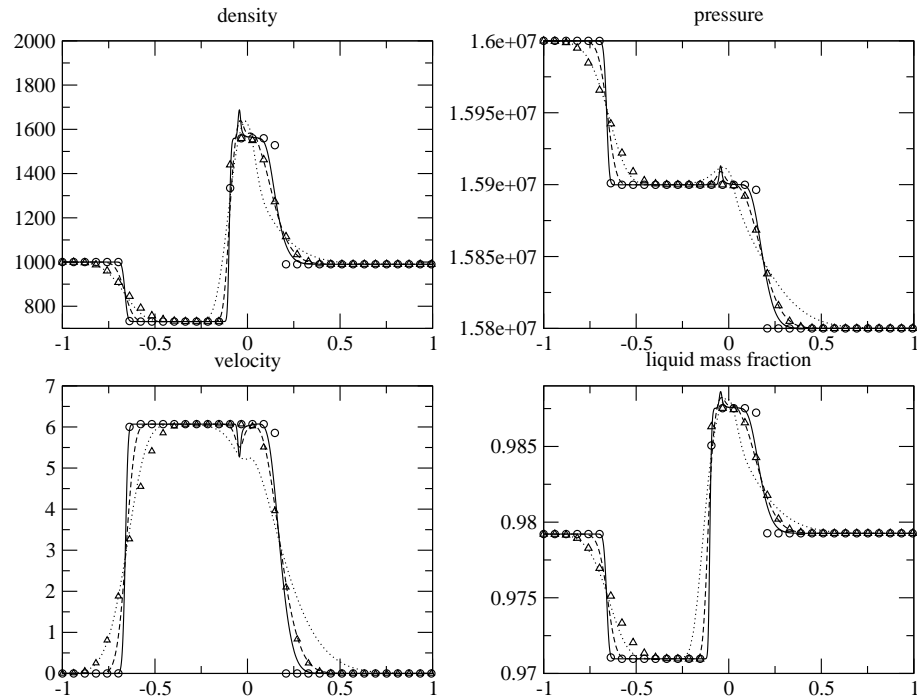


FIG. D.14 – Constant time scale τ_0^2 . The initial discontinuity is in the HEM domain. A shock wave travels to the right and goes through the coupling interface ($x = 0$). A rarefaction wave travels to the left. A contact discontinuity travels to the right but is still on the left of the coupling interface. Circles=HEM 10000 cells, triangles=HRM 10000 cells, line=HEM/HRM 10000 cells, dashed line=HEM/HRM 500 cells, dot line=HEM/HRM 100 cells.

D.3.2 A rarefaction wave traveling from HEM domain to HRM domain

domain :	HEM	HEM	HRM
U	0	0	0
P	158e5	160e5	160e5
ρ	990	1000	1000
C	none	none	0.979212418
C_{eq}	0.979261526	0.979212418	0.979212418

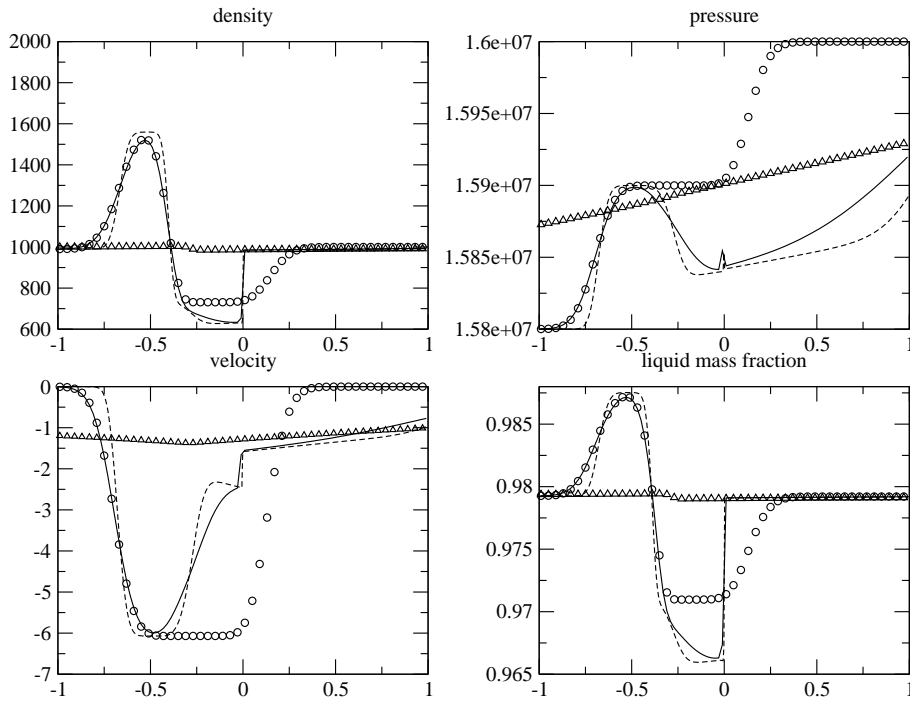


FIG. D.15 – Constant time scale τ_0^1 . The initial discontinuity is in the HEM domain. A rarefaction wave travels to the right and goes through the coupling interface ($x = 0$). A shock wave travels to the left. A contact discontinuity travels to the left. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, There are no results for HEM/HRM 500 cells and 10000 cells because the computed solution goes out from D_{HRM} .

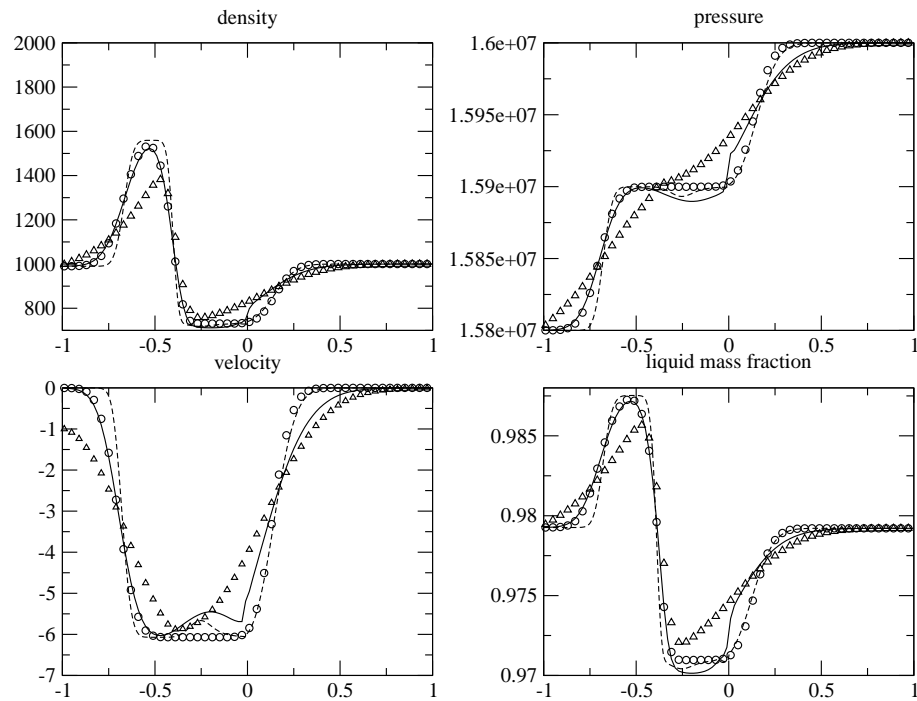


FIG. D.16 – Constant time scale τ_0^2 . The initial discontinuity is in the HEM domain. A rarefaction wave travels to the right and goes through the coupling interface ($x = 0$). A shock wave travels to the left. A contact discontinuity travels to the left. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, dashed line=HEM/HRM 500 cells.

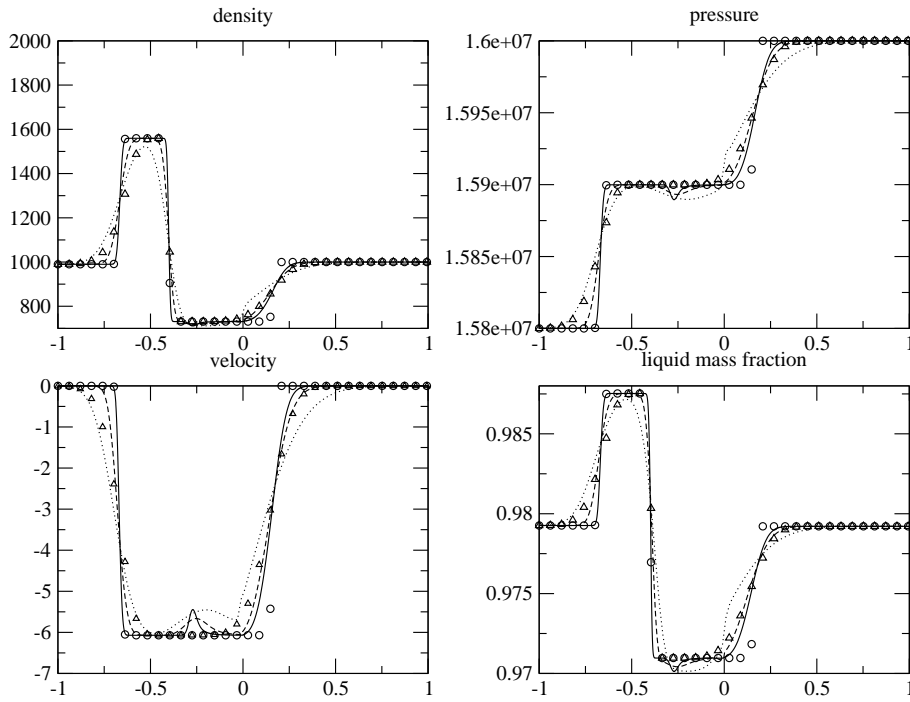


FIG. D.17 – Constant time scale τ_0^2 . The initial discontinuity is in the HEM domain. A rarefaction wave travels to the right and goes through the coupling interface ($x = 0$). A shock wave travels to the left. A contact discontinuity travels to the left. Circles=HEM 10000 cells, triangles=HRM 10000 cells, line=HEM/HRM 10000 cells, dashed line=HEM/HRM 500 cells, dot line=HEM/HRM 100 cells.

D.3.3 A shock wave traveling from HRM domain to HEM domain

domain :	HEM	HRM	HRM
U	0	0	0
P	158e5	158e5	160e5
ρ	990	990	1000
C	none	0.979261526	0.979212418
C_{eq}	0.979261526	0.979261526	0.979212418

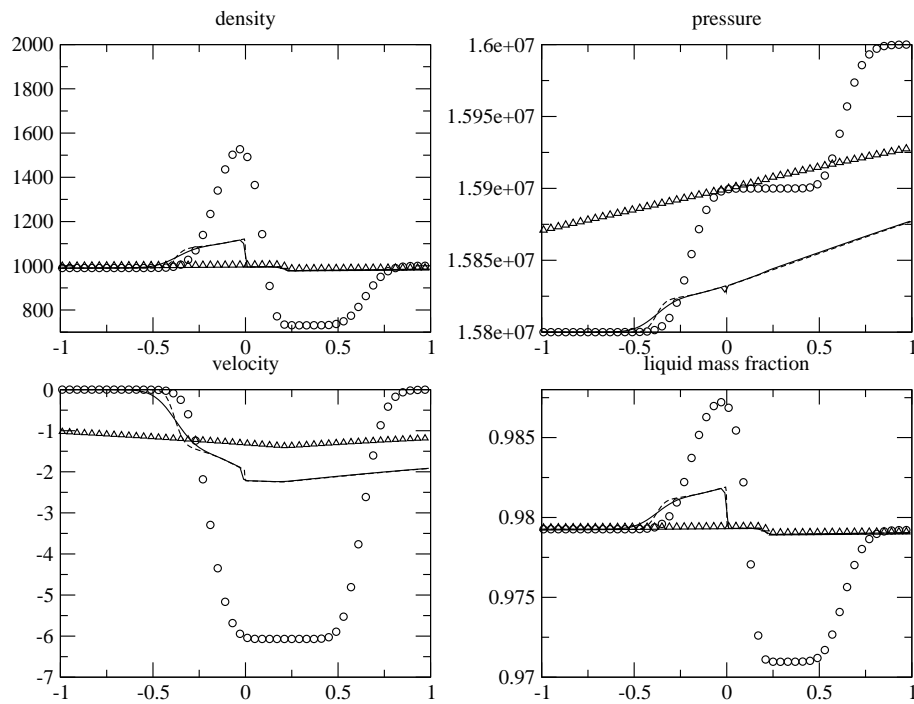


FIG. D.18 – Constant time scale τ_0^1 . The initial discontinuity is in the HRM domain. A shock wave travels to the left and goes through the coupling interface ($x = 0$). A rarefaction wave travels to the right. A contact discontinuity travels to the left but is still on the right of the coupling interface. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, There are no results for HEM/HRM 10000 cells because the computed solution goes out from D_{HRM} .

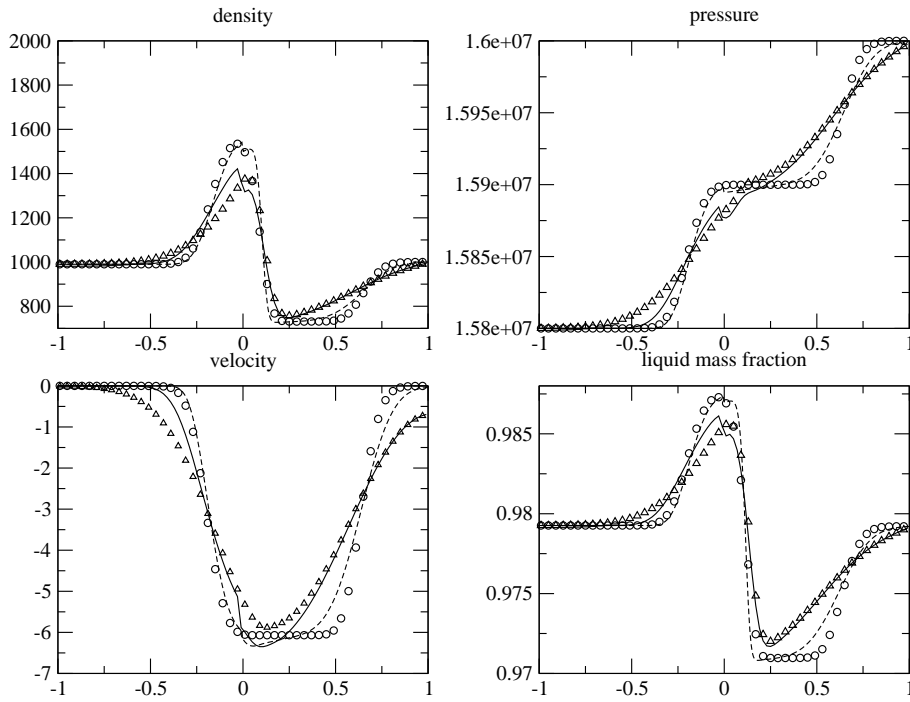


FIG. D.19 – Constant time scale τ_0^2 . The initial discontinuity is in the HRM domain. A shock wave travels to the left and goes through the coupling interface ($x = 0$). A rarefaction wave travels to the right. A contact discontinuity travels to the left but is still on the right of the coupling interface. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, dashed line=HEM/HRM 500 cells.

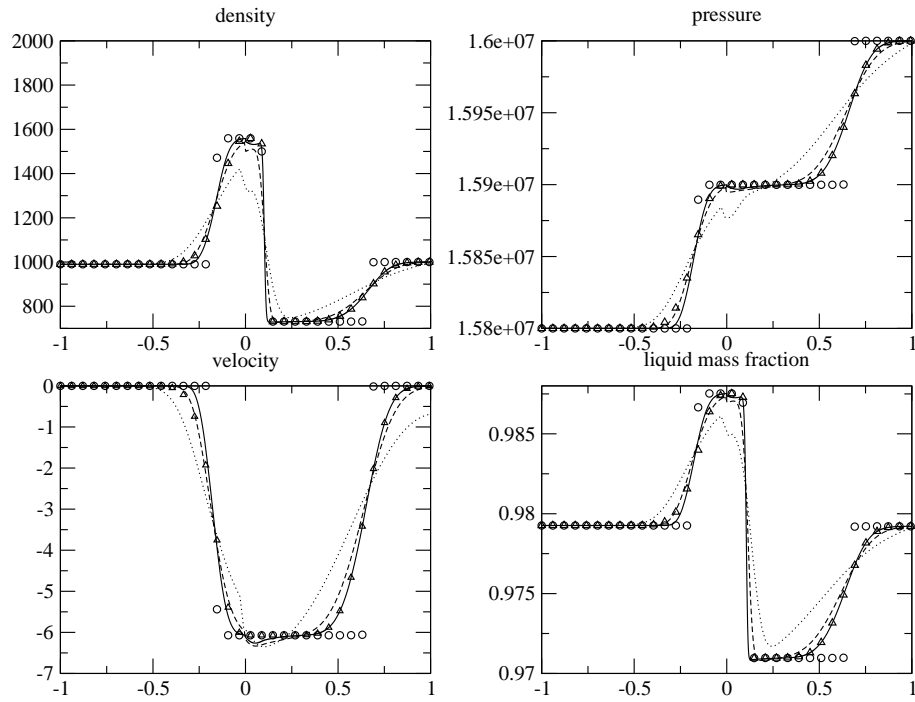


FIG. D.20 – Constant time scale τ_0^2 . The initial discontinuity is in the HRM domain. A shock wave travels to the left and goes through the coupling interface ($x = 0$). A rarefaction wave travels to the right. A contact discontinuity travels to the left but is still on the right of the coupling interface. Circles=HEM 10000 cells, triangles=HRM 10000 cells, line=HEM/HRM 10000 cells, dashed line=HEM/HRM 500 cells, dot line=HEM/HRM 100 cells.

D.3.4 A rarefaction wave traveling from HRM domain to HEM domain

domain :	HEM	HRM	HRM
U	0	0	0
P	160e5	160e5	158e5
ρ	1000	1000	990
C	none	0.979212418	0.979261526
C_{eq}	0.979212418	0.979212418	0.979261526

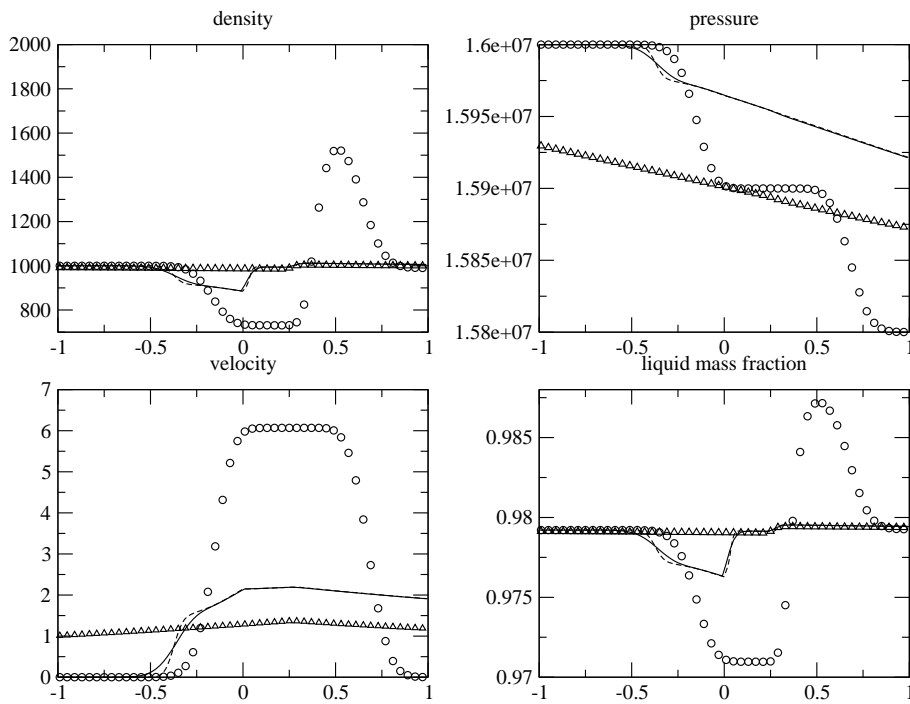


FIG. D.21 – Constant time scale τ_0^1 . The initial discontinuity is in the HRM domain. A rarefaction wave travels to the left and goes through the coupling interface ($x = 0$). A shock wave travels to the right. A contact discontinuity travels to the right. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, There are no results for HEM/HRM 10000 cells because the computed solution goes out from D_{HRM} .

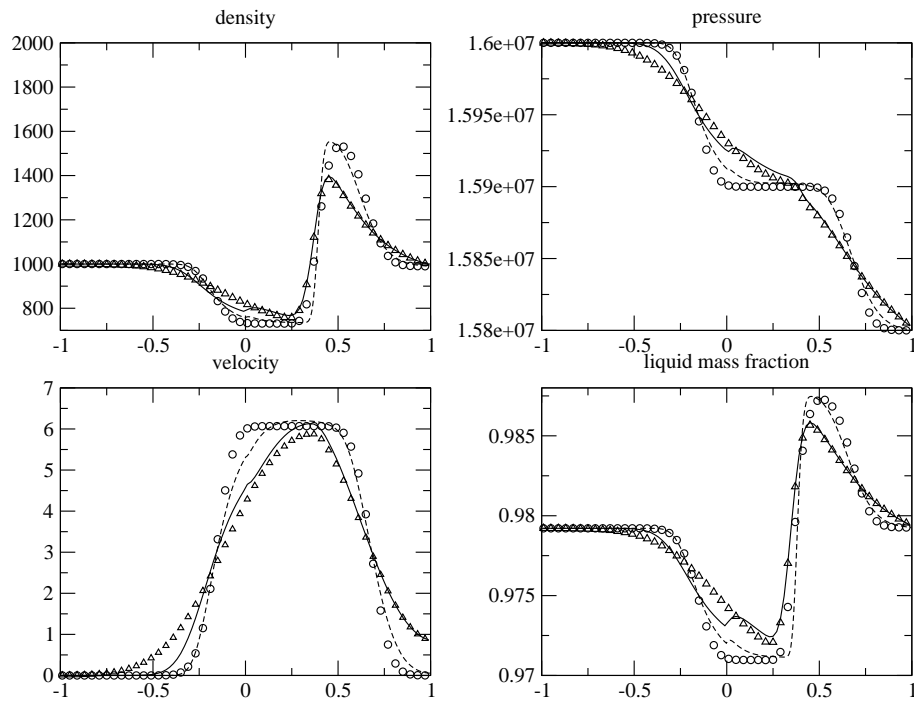


FIG. D.22 – Constant time scale τ_0^2 . The initial discontinuity is in the HRM domain. A rarefaction wave travels to the left and goes through the coupling interface ($x = 0$). A shock wave travels to the right. A contact discontinuity travels to the right. Circles=HEM 100 cells, triangles=HRM 100 cells, line=HEM/HRM 100 cells, dashed line=HEM/HRM 500 cells.

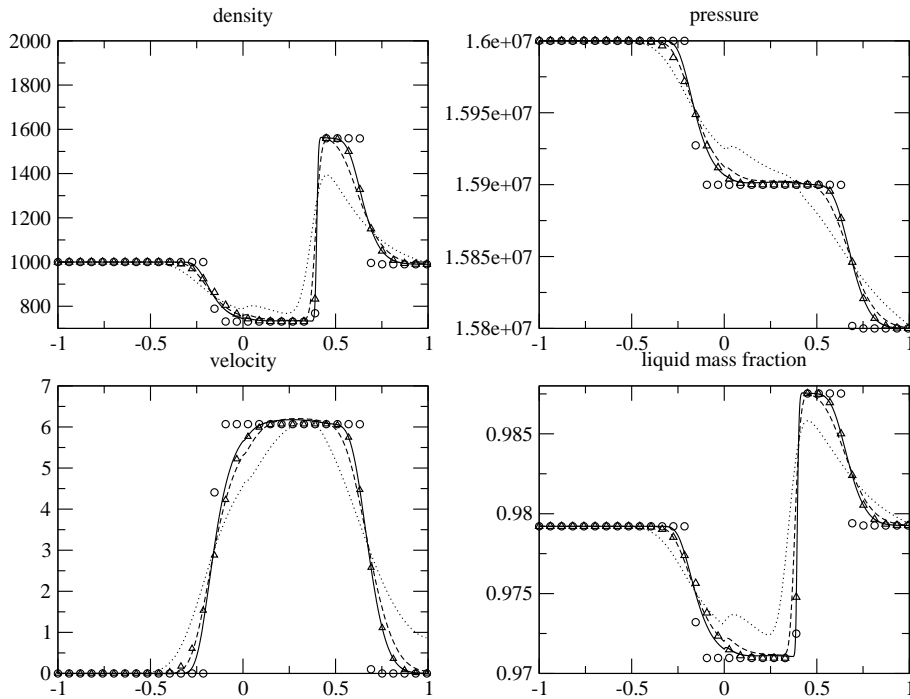


FIG. D.23 – Constant time scale τ_0^2 . The initial discontinuity is in the HRM domain. A rarefaction wave travels to the left and goes through the coupling interface ($x = 0$). A shock wave travels to the right. A contact discontinuity travels to the right. Circles=HEM 10000 cells, triangles=HRM 10000 cells, line=HEM/HRM 10000 cells, dashed line=HEM/HRM 500 cells, dot line=HEM/HRM 100 cells.

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TITRE**COUPLAGE INTERFACIAL INSTATIONNAIRE DE MODÈLES DIPHASIQUES****RESUME**

Le circuit primaire d'une centrale nucléaire est composé d'un ensemble d'éléments très différents (cuve, coeur, réseau de conduite ...). A chacun de ces éléments correspond actuellement un ou plusieurs codes de calcul spécifiques basés sur des systèmes d'équations aux dérivées partielles spécifiques. Afin de permettre la simulation des écoulements diphasiques dans l'ensemble du circuit primaire, il faut envisager de coupler ces différents codes. L'approche proposée dans ce travail de thèse est de coupler les codes grâce à un échange d'information interfaciale instationnaire. Des flux numériques sont calculés au niveau des interfaces de couplage et servent de conditions aux limites à chacun des codes. Les méthodes permettant le calcul des flux de couplage sont dérivées du formalisme de Greenberg-Leroux proposé dans le cadre du décentrement des termes sources des systèmes hyperboliques non-homogènes stationnaires, et font intervenir un modèle d'interface. Trois cas de couplage ont été examinés :

- le couplage du système des équations d'Euler en dimension un et deux ;
- le couplage de deux modèles diphasiques homogènes distincts ;
- le couplage d'un modèle homogène à quatre équations et du modèle bi-fluide standard.

Mots clés : Couplage interfacial, modèles diphasiques, Volumes Finis, systèmes hyperboliques, écoulements instationnaires

TITLE**UNSTEADY INTERFACIAL COUPLING OF TWO-PHASE FLOW MODELS****ABSTRACT**

The primary coolant circuit in a nuclear power plant contains several distinct components (vessel, core, pipes,...). For all components, specific codes based on the discretization of partial differential equations have already been developed. In order to obtain simulations for the whole circuit, the interfacial coupling of these codes is required. The approach examined within this work consists in coupling codes by providing unsteady information through the coupling interface. The numerical technique relies on the use of an interface model, which is combined with the basic strategy that was introduced by Greenberg and Leroux in order to compute approximations of steady solutions of non-homogeneous hyperbolic systems. Three different coupling cases have been examined:

- the coupling of a one-dimensional Euler system with a two-dimensional Euler system;
- the coupling of two distinct homogeneous two-phase flow models;
- the coupling of a four-equation homogeneous model with the standard two-fluid model.

Keywords : Interfacial coupling, two-phase flow models, Finite Volumes, hyperbolic systems, unsteady flows.

Discipline - Spécialité Doctorale : Mathématiques appliquées.

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