Numerical Coupling of Two-Phase Flows

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> **Abstract.** We present numerical methods to simulate a two-phase flow that is described by a Homogeneous Equilibrium Model on the left of a fictious fixed interface and by a Homogeneous Relaxation Model on the right of it. No *a priori* information at the coupling interface is provided for the flow. Such a problem appears in industrial simulation platforms, where different codes are used to treat specific sub-domains of complex systems. We propose several coupling techniques that allow to efficiently simulate the flow which fulfill a set of physical constraints that must be imposed at the interface.

Key words: Two-phase flow, coupling of models, hyperbolic system, finite volume methods.

1 Introduction

This paper deals with the numerical coupling of two models of compressible homogeneous twophase flows, through an fixed interface, located at x = 0. The space domain is separated in two regions, $D^- := \mathbb{R}^*_{-}$ and $D^+ := \mathbb{R}^*_{+}$, in which the flow is governed by different systems of PDEs. The model in D^- (respectively in D^+) is indexed by L (resp. by R) and the global problem takes the following form:

$$\partial_t \mathbf{u}_L + \partial_x \mathbf{f}_L(\mathbf{u}_L) = 0, \qquad t > 0, x \in D^-, \qquad (L)$$

$$\partial_t \mathbf{u}_R + \partial_x \mathbf{f}_R(\mathbf{u}_R) = \mathbf{s}_R(\mathbf{u}_R), \qquad t > 0, x \in D^+,$$
(R)

with appropriate initial conditions. Though both models aim at represent the same physical phenomenon, they can be different. Such a situation often occurs when two codes with different models and solvers are used to simulate two continguous parts of a flow.

Here, the two models govern a flow of water, which can be present under its vapor form or in under its liquid form. Moreover, both models takes into account for phase transition. The models we consider belong to the class of homogeneous models: the mixture of vapor and liquid water

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follows the compressible non isothermal Euler equations. The difference between the models (L) and (R) comes from their thermodynamic law which describes the phase transition.

For the model (L), the thermodynamic equilibrium (i.e. the equality of temperatures, pressures and chemical potentials) is assumed to be fulfilled for every $(t, x) \in \mathbb{R}_+ \times D^-$. Hence, the phenomenon of phase transition is completely involved in the equation of state of the fluid. Several models of equation of state can be used, the most popular being the one proposed by Van der Waals at the end of the 19th century. Here, we use a simpler one, proposed for instance in [10] and [4], which has the advantage to provide a hyperbolic system of PDEs. This model is called the *Homogeneous Equilibrum Model* (HEM).

For the model (R), only the thermal and mechanical equilibria are instantaneously verified (i.e. the equality of temperatures and pressures), whereas the difference of the chemical potentials is assumed to vanish only when $t \to \infty$. This behaviour is modeled by a PDE for the mass fraction of the vapor phase, which involves a relaxation term based on the difference of the chemical potentials. This relaxation term vanishes when the thermodynamic equilibrium is obtained. This model is referred as the Homogeneous Relaxation Model (HRM).

We will suppose here that HEM is the formal limit of HRM, when the relaxation process becomes instantaneous. In spite of the thermodynamical compatibility of the models, their coupling is not obvious as soon as the flow is not at thermodynamical equilibrium in the domain of HRM, that is D^+ . Indeed, it is easy to show that different solutions to the coupling problem (L-R) can be obtained according to the model of coupling we impose at the interface x = 0(see [3]). The models of coupling that we investigate here differ by their properties:

- conservation of mass, momentum and total energy,
- conservation of mass, momentum and ability to keep unchanged unsteady contact discontinuities,
- continuity of density, momentum and total energy at the coupling interface,
- conservation of mass and total energy and continuity of the specific enthalpy at the coupling interface.

Moreover, since both models are hyperbolic systems, these coupling conditions must be understood in a weak sense (in the same way as boundary conditions, see [2] and [6]). For the theoritical point of view, we refer to [7] and [8].

The aim of this paper is to propose some numerical methods of coupling, in the frame of Finite Volume schemes, in agreement with the models of coupling mentioned above. In fact, two class of methods are presented. The first one allow us to obtain a conservative numerical method for mass, momentum and total energy and is based on the use of an extended model and of a relaxation method. The other one may be seen as an adaptation of the numerical methods presented in [9] and in [1]. This method enables us to approximate several models of coupling, giving at the numerical level the weak continuity of some variables. Note that all these numerical methods of coupling are independent from the numerical schemes used in each domain, only the numerical fluxes at the interface are modified.

In the second section of this paper are presented the two models, HEM and HRM, and their main properties. The next section deals with the numerical methods of coupling and their ability to approximate the models of coupling. The last section is devoted to numerical results, allowing to compare the behaviour of the different numerical methods.

2 Governing equations

We detail in this section the two models we aim at coupling, HEM and HRM, and the mathematical problem of coupling.

2.1 The Homogeneous Equilibrium Model

This model describes a two-phase flow, composed by water under its vapor (phase 1) or its liquid form (phase 2). This mixture is governed by the following set of PDEs:

$$\partial_t \rho + \partial_x \rho u = 0,$$

$$\partial_t \rho u + \partial_x (\rho u^2 + p) = 0,$$

$$\partial_t \rho E + \partial_x (\rho E + p) u = 0,$$

(1)

where ρ , u and p respectively denote the density, the velocity and the pressure of the mixture, and the total energy E is the sum of the specific energy and the kinetic energy: $E = \varepsilon + u^2/2$. We will use in the following the condensed form (L), where \mathbf{u}_L and \mathbf{f}_L find a clear definition from system (1). Since the thermodynamical equilibrium is assumed to be instantaneously fulfilled, the whole thermodynamical behaviour is involved in the definition of the equation of state. Here, we use the model developed in [10] and in [4], which leads to the following definition of the pressure:

$$p = p^{HEM}(\rho, \varepsilon) := \begin{cases} (\gamma_1 - 1)\rho\varepsilon & \text{if } \rho \le \rho_1^\star, \\ (\gamma_1 - 1)\rho_1^\star \varepsilon & \text{if } \rho_1^\star < \rho < \rho_2^\star, \\ (\gamma_2 - 1)\rho\varepsilon & \text{if } \rho \ge \rho_2^\star, \end{cases}$$
(2)

where the two adiabatic coefficients γ_1 and γ_2 verify $1 < \gamma_2 < \gamma_1$ and where the two constant densities ρ_1^* and ρ_2^* are defined by

$$\rho_1^{\star} = \frac{1}{e} \left(\frac{\gamma_2 - 1}{\gamma_1 - 1} \right)^{\frac{\gamma_2}{\gamma_2 - \gamma_1}} \quad \text{and} \quad \rho_2^{\star} = \frac{1}{e} \left(\frac{\gamma_2 - 1}{\gamma_1 - 1} \right)^{\frac{\gamma_1}{\gamma_2 - \gamma_1}}.$$

Note that $(\gamma_1 - 1)\rho_1^* = (\gamma_2 - 1)\rho_2^*$. This pressure law is only \mathcal{C}^0 when the density is equal to ρ_1^* or ρ_2^* . Nonetheless, this system is hyperbolic over the set

$$\Omega^{HEM} := \left\{ \mathbf{u}_L := (\rho, \rho u, \rho E) \in \mathbb{R}^3 / \rho > 0, \rho \neq \rho_1^*, \rho \neq \rho_2^*, \varepsilon > 0 \right\}$$

and the eigenvalues associated with the system (1) are

$$\lambda_1(\mathbf{u}_L) = u - c^{HEM}(\mathbf{u}_L) < \lambda_2(\mathbf{u}_L) = u < \lambda_3(\mathbf{u}_L) = u + c^{HEM}(\mathbf{u}_L),$$

where the sound speed c^{HEM} is defined by

$$\left(c^{HEM}(\mathbf{u}_L) \right)^2 := \begin{cases} \gamma_1(\gamma_1 - 1)\varepsilon & \text{if } 0 < \rho \le \rho_1^\star, \\ (\gamma_1 - 1)^2(\rho_1^\star)^2 \varepsilon / \rho^2 & \text{if } \rho_1^\star < \rho < \rho_2^\star, \\ \gamma_2(\gamma_2 - 1)\varepsilon & \text{if } \rho \ge \rho_2^\star. \end{cases}$$

Let us also emphasize that, due to the definition (2) of the pressure law p^{HEM} , the first and the third fields can be composed of multiple waves [11].

2.2 The Homogeneous Relaxation Model

This model includes a relaxation term which comes from the difference of the chemical potentials of the liquid phase and of the vapor phase. Defining m_1 as the partial density of the vapor, the homogeneous relaxation model reads

$$\partial_t m_1 + \partial_x m_1 u = \lambda_0 (m_1^*(\rho) - m_1),$$

$$\partial_t \rho + \partial_x \rho u = 0,$$

$$\partial_t \rho u + \partial_x (\rho u^2 + p) = 0,$$

$$\partial_t \rho E + \partial_x (\rho E + p) u = 0,$$

(3)

where λ_0 is the relaxation parameter and m_1^{\star} the equilibrium partial density of vapor, defined by

$$m_1^*(\rho) = \begin{cases} \rho, & \text{if } \rho \le \rho_1^*, \\ \rho_1^* \frac{\rho - \rho_2^*}{\rho_1^* - \rho_2^*}, & \text{if } \rho_1^* < \rho < \rho_2^*, \\ 0, & \text{if } \rho \ge \rho_2^*. \end{cases}$$
(4)

The equilibrium $m_1 = m_1^*$ is equivalent to the equality of the chemical potentials. The equation of state is now

$$p = p^{HRM}(\rho, \varepsilon, m_1) := ((\gamma_1 - 1)m_1 + (\gamma_2 - 1)(\rho - m_1))\varepsilon$$
(5)

and verifies the compatibility relation with HEM:

$$p^{HRM}(\rho,\varepsilon,m_1^{\star}(\rho)) = p^{HEM}(\rho,\varepsilon), \quad \forall \rho > 0, \forall \varepsilon > 0.$$
(6)

(This model corresponds to the model (R), with clear definitions of \mathbf{u}_R , \mathbf{f}_R and \mathbf{s}_R .) This model is hyperbolic over the set

$$\Omega^{HRM} := \left\{ \mathbf{u} := (m_1, \rho, \rho u, \rho E) \in \mathbb{R}^4 / \rho > 0, 0 < m_1 < \rho, \varepsilon > 0 \right\}$$

The eigenvalues of the differential part of the system are

$$\lambda_1(\mathbf{u}_R) = u - c^{HRM}(\mathbf{u}_R) < \lambda_2(\mathbf{u}_R) = \lambda_3(\mathbf{u}_R) = u < \lambda_4(\mathbf{u}_R) = u + c^{HRM}(\mathbf{u}_R),$$

where the sound speed c^{HRM} is

$$\left(c^{HRM}(\mathbf{u}_R)\right)^2 := B(m_1,\rho)(1+B(m_1,\rho))\varepsilon,$$

with $B(m_1, \rho) = ((\gamma_1 - 1)m_1 + (\gamma_2 - 1)(\rho - m_1))/\rho$. Note that if $\lambda_0 = 0$, this model is a classical multicomponent model, with the isobaric-isothermal closure.

2.3 The models of coupling

We focus now on the mathematical modeling of the coupling problem at $\{x = 0\}$. Independently of the model of coupling, the problem is composed by the two systems

$$\partial_t \mathbf{u}_L + \partial_x \mathbf{f}_L(\mathbf{u}_L) = 0, \qquad t > 0, x \in D^-, \tag{L}$$

$$\partial_t \mathbf{u}_R + \partial_x \mathbf{f}_R(\mathbf{u}_R) = \mathbf{s}_R(\mathbf{u}_R), \qquad t > 0, x \in D^+,$$
(R)

and by the initial conditions

$$\mathbf{u}_L(x,0) = \mathbf{u}_L^0(x), \quad x \in D^-, \mathbf{u}_R(x,0) = \mathbf{u}_R^0(x), \quad x \in D^+,$$
(7)

where $\mathbf{u}_{L}^{0} \in \Omega^{HEM}$ and $\mathbf{u}_{R}^{0} \in \Omega^{HRM}$ are given. It remains to specify the model of coupling at the interface, that is the connection between $\mathbf{u}_{L}(0^{-},t)$ and $\mathbf{u}_{R}(0^{+},t)$, which are the traces of the solution at the interface of coupling. In order to simplify the presentation, suppose in the following that $\mathbf{s}_{R} \equiv 0$.

2.3.1 The flux coupling

We present first a model of coupling leading to solutions whose mass, momentum and total energy are conserved. Using the compatibility relation (6), we can define the global system

$$\partial_t m_1 + \partial_x m_1 u = \mu(x)(m_1^*(\rho) - m_1),$$

$$\partial_t \rho + \partial_x \rho u = 0,$$

$$\partial_t \rho u + \partial_x (\rho u^2 + p) = 0,$$

$$\partial_t \rho E + \partial_x (\rho E + p) u = 0,$$

$$p = p^{HRM}(\rho, \varepsilon, m_1),$$

(8)

for $(x,t) \in \mathbb{R} \times \mathbb{R}^*_+$, with

$$\mu(x) = \begin{cases} +\infty & \text{if } x < 0, \\ 0 & \text{if } x > 0. \end{cases}$$

This global model is formally equivalent to HEM in D^- and to HRM in D^+ . Besides, its solutions fulfill the conservation of mass, momentum and total energy. Such a model can be interpreted as imposing the equality between $\mathbf{f}_L(\mathbf{u}_L(0^-, t))$ and the three last components of $\mathbf{f}_R(\mathbf{u}_R(0^-, t))$, for all t > 0.

2.3.2 The intermediate state coupling

Here, the intermediate state coupling lies on some variables that we try to maintain constant through the interface $\{x = 0\}$. The mathematical framework has been defined in [7] and [8]. Assume first of all that we would like to impose the continuity of ρ , ρu and ρE through the coupling interface. The model developed in [8] may be roughly resumed as follows in our problem:

- In x = 0, the model (L) is supplemented by a Dirichlet boundary condition given by three last components of $\mathbf{u}_R(0^+, t)$.
- In x = 0, the model (R) is supplemented by a Dirichlet boudary condition given by $\mathbf{u}_L(0^-, t)$ and $m_1^*(\rho(0^-, t))$.

Since we are dealing with hyperbolic systems, these boundary conditions must be understood in a weak way (which is not precised here, see [6], [8] and [3] for more details). Therefore, as soon as possible, the continuity of ρ , ρu and ρE is achieved.

This method is not restricted to the conservative variables, the extension to different variables is quite natural. Instead of imposing the conservative variables at each boundary, other variables are provided as boundary conditions.

Three different sets of variables are tested: $(\rho, \rho u, \rho E)$, $(\rho, \rho u, p)$ and $(\rho, \rho u, p+\varepsilon/\rho)$. When the continuity of the transmitted variable is achieved, note that the associated solution is conservative in: ρ for the first coupling, ρ and ρu for the second coupling, ρ and ρE for the last coupling.

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3 Numerical methods of coupling

We present now different numerical methods, enabling to approximate the different stategies of coupling defined above. We restrict to the frame of Finite Volume methods and, in order to symplify the presentation, only three-point schemes are considered. Let Δx and Δt be the space step and the time step. Let us note the cells of the mesh $C_{j+1/2} = (j\Delta x, (j+1)\Delta x), j \in \mathbb{Z}$. We aim at define the approximations

$$\left((\mathbf{u}_L)_{j-1/2}^n \right)_{j \le 0, n > 0} \in \Omega^{HRM},\tag{9}$$

and

$$\left(\left(\mathbf{u}_R \right)_{j+1/2}^n \right)_{j \ge 0, n > 0} \in \Omega^{HRM},\tag{10}$$

of the solutions \mathbf{u}_L and \mathbf{u}_R . We assume that the numerical schemes in each domain are given:

$$(\mathbf{u}_L)_{j-1/2}^{n+1} = (\mathbf{u}_L)_{j-1/2}^n - \frac{\Delta t}{\Delta x} ((\mathbf{g}_L)_j^n - (\mathbf{g}_L)_{j-1}^n), \quad j < 0, n > 0,$$
(11)

$$(\mathbf{u}_R)_{j+1/2}^{n+1} = (\mathbf{u}_R)_{j+1/2}^n - \frac{\Delta t}{\Delta x} \left((\mathbf{g}_R)_{j+1}^n - (\mathbf{g}_R)_j^n \right), \quad j > 0, n > 0,$$
(12)

where

$$(\mathbf{g}_L)_j^n = \mathbf{g}_L((\mathbf{u}_L)_{j-1/2}^n, (\mathbf{u}_L)_{j+1/2}^n), \quad (\mathbf{g}_R)_j^n = \mathbf{g}_R((\mathbf{u}_R)_{j-1/2}^n, (\mathbf{u}_R)_{j+1/2}^n)$$
(13)

where $\mathbf{g}_L(.,.)$ and $\mathbf{g}_R(.,.)$ are two classical numerical fluxes. Therefore, in order to compute $(\mathbf{u}_L)_{-1/2}^n$ and $(\mathbf{u}_R)_{+1/2}^n$, we must define the numerical fluxes at the interface of coupling: $(\mathbf{g}_L)_0^n$ and $(\mathbf{g}_R)_0^n$.

3.1 The numerical flux coupling

We first focus on defining the numerical fluxes $(\mathbf{g}_L)_0^n$ and $(\mathbf{g}_R)_0^n$ related to the flux coupling.

These numerical fluxes are computed using the global system (8), using a two-step approximation: the first step consists in solving the PDE part of (8) (i.e. system (8) with $\mu \equiv 0$) while the second step consists in the approximation of the source term. More precisely, let us define

$$(\mathbf{u}_L^{\star})_{-1/2}^n := (m_1^{\star}(\rho_{-1/2}^n), (\mathbf{u}_L)_{-1/2}^n),$$

then, using the previous two-step algorithm, we may finally obtain

$$(\mathbf{g}_R)_0^n := \mathbf{g}_R((\mathbf{u}_L^{\star})_{-1/2}^n, (\mathbf{u}_R)_{-1/2}^n)$$
(14)

and

$$\left((\mathbf{g}_L)_0^n \right)^{(i)} := \left((\mathbf{g}_R)_0^n \right)^{(i+1)}, \quad i = 1, 2, 3,$$
(15)

where the notation $(\mathbf{v})^{(i)}$ denotes de *i*-th component of the vector \mathbf{v} . By construction, this method is conservative with respect to the mass, momentum and total energy.

3.2 The numerical intermediate state coupling

The numerical method we propose is similar to the numerical methods proposed in [9] and [1]. The cornerstone of this method is the use of two fictitious states, $(\overline{\mathbf{u}_L})_{+1/2}^n \in \Omega^{HEM}$ and $(\overline{\mathbf{u}_R})_{-1/2}^n \in \Omega^{HRM}$. Then, the numerical fluxes at the interface are defined by

$$(\mathbf{g}_L)_0^n := \mathbf{g}_L((\mathbf{u}_L)_{-1/2}^n, (\overline{\mathbf{u}_L})_{+1/2}^n)), \tag{16}$$

$$(\mathbf{g}_R)_0^n := \mathbf{g}_R((\overline{\mathbf{u}_R})_{-1/2}^n, (\mathbf{u}_R)_{+1/2}^n)).$$

$$(17)$$

According to the coupling we want to obtain, the definition of the two fictitious states will be different.

Assume that the theoritical intermediate state coupling (and thus the Dirichlet boundary conditions) is defined with the help of two changes of variable $\phi_L : \Omega^{HEM} \mapsto \mathbb{R}^3$ and $\phi_R : \Omega^{HRM} \mapsto \mathbb{R}^4$, such that we would like to obtain the following coupling condition:

$$\phi_L[\mathbf{u}_L(0^-, t)]^{(i)} = \phi_R[\mathbf{u}_R(0^-, t)]^{(i+1)}, \quad i = 1, 2, 3.$$
(18)

Therefore, the two fictitious states are given by

$$(\overline{\mathbf{u}_L})_{+1/2}^n := \phi_L^{-1}[(\phi_R[(\mathbf{u}_R)_{+1/2}^n])^{(2,3,4)}]$$
(19)

$$(\overline{\mathbf{u}_R})_{-1/2}^n := \phi_R^{-1}[(m_1^*(\rho_{-1/2}^n), \phi_L[(\mathbf{u}_L)_{-1/2}^n])].$$
(20)

Here, we use three different couples of change of variable (ϕ_L, ϕ_R) , according to the coupling model we want to prescribe:

• Continuity of $(\rho, \rho u, \rho E)$:

$$\phi_L[(\rho, \rho u, \rho E)] := (\rho, \rho u, \rho E),$$

$$\phi_R[(m_1, \rho, \rho u, \rho E)] := (m_1, \rho, \rho u, \rho E).$$

• Continuity of $(\rho, \rho u, p)$:

$$\phi_L[(\rho, \rho u, \rho E)] := (\rho, \rho u, p^{HEM}(\rho, E - u^2/2)),$$

$$\phi_R[(m_1, \rho, \rho u, \rho E)] := (m_1, \rho, \rho u, p^{HRM}(\rho, E - u^2/2, m_1)).$$

• Continuity of $(\rho, \rho u, \varepsilon + p/\rho)$:

$$\phi_L[(\rho,\rho u,\rho E)] := (\rho,\rho u, p^{HEM}(\rho, E - u^2/2) + (E - u^2/2)),$$

$$\phi_R[(m_1,\rho,\rho u,\rho E)] := (m_1,\rho,\rho u, (E - u^2/2) + p^{HRM}(\rho, E - u^2/2, m_1)/\rho).$$

This numerical method of coupling aims at providing, whenever possible, the continuity of the suitable variables. Nonetheless, since two different numerical fluxes are used at the coupling interface, the global method cannot be strictly conservative, even if the coupling model imposes the continuity of the flux of a variable.

4 Numerical results

The numerical fluxes \mathbf{g}_L and \mathbf{g}_R which are used here are those associated with a Lagrange-Projection scheme (see for instance [5] for a description of this scheme).

As noted before, if the flow is at equilibrium in D^+ , the global model is formally HEM. Therefore, all the coupling models and all the numerical methods of coupling provide the same solution. That's why we choose in the following test case to initialize m_1 and ρ in D^+ such that $m_1 \neq m_1^*(\rho)$. The initial condition is the following:

$$\begin{aligned} &x \in (-1/2,0), \quad \mathbf{u}_L(x,0) = (\rho^0, u^0, \rho((u^0)^2/2 + \varepsilon^{HEM}(\rho^0, p^0))), \\ &x \in (0,+1/2), \quad \mathbf{u}_R(x,0) = (\rho^0, u^0, \rho((u^0)^2/2 + \varepsilon^{HRM}(\rho^0, p^0, m_1^0)), m_1^0), \end{aligned}$$

with $\rho^0 = 1$, $u^0 = -1/2$, $p^0 = 1$ and $m_1^0 = 1$. The adiabatic coefficients are $\gamma_1 = 1.6$ and $\gamma_2 = 1.4$, so that $\rho_1^* \approx 0.6131$ and $\rho_2^* \approx 0.9197$ and thus $m_1^0 \neq m_1^*(\rho^0)$. Moreover, since the density, the velocity and the pressure are constant in the whole domain (-1/2, +1/2), the intermediate state coupling based on the variable (ρ, u, p) must let the initial data unchanged.

The different numerical results are plotted at t = 0.2 and with $\lambda_0 = 0$ for HRM. The mesh is uniform and composed of 500 cells and the Courant number is 0.4.



Figure 1: Density ρ with the different coupling methods.

In Figs. 1, 2, 3 and 4 are respectively plotted the density, the velocity, the pressure and the fraction of vapor (i.e. m_1/ρ). It can be seen in Figs. 1, 2 and 3 that the coupling based on $(\rho, \rho u, p)$ exactly preserves the density, the velocity and the pressure constant. The three other coupling methods introduce waves and intermediate states. Besides, the coupling methods based on $(\rho, \rho u, \rho E)$ and $(\rho, \rho u, \varepsilon + p/\rho)$ do not provide a solution with the appropriate variable continuous at the interface. This is of course due to the fact that $m_1^0 \neq m_1^*(\rho^0)$, since the thermodynamic law is different on each part of the interface of coupling.

It is also worth noting that the solutions provided by the coupling methods based on the variables $(\rho, \rho u, \rho E)$ and $(\rho, \rho u, \varepsilon + p/\rho)$ contain a mixture zone in D^- (see Fig. 4). Note also in Fig. 3 that the two latter coupling methods and the flux coupling make a boundary layer appear at the interface of coupling.

It has been shown by this simple numerical example that the solutions provided by the coupling of two different models strongly depend on the model of coupling which is used at the interface of coupling.

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Figure 2: Velocity u with the different coupling methods.



Figure 3: Pressure p with the different coupling methods.



Figure 4: Fraction of vapor m_1/ρ with the different coupling methods.

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