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NUMERICAL SIMULATION OF LOW MACH NUMBER LIQUID GAS FLOWS

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ABSTRACT

This work is devoted to the numerical simulation of liquid-gas flows. The liquid phase is considered as incompressible, while the gas phase is treated as compressible in the low Mach number approach. We present a model and a numerical method aimed at the computation of such two-phase flows. The numerical model uses a lagrangian front-tracking method to deal with the interface. To validate our model, we present preliminary results in the 1D case of a heated enclosure, inside which a liquid zone is inserted between two gaseous zones.

INTRODUCTION

This work is devoted to the numerical simulation of liquid-gas flows with realistic physical properties and high density ratios between the phases. For confined flows (as is often the case in nuclear engineering or microfluidic applications), the variations of the thermodynamic pressure in the gaseous phase play an important role and must be taken into account. This means that the gaseous phase must be treated as a compressible fluid. However, in most of the applications the velocities in the gas are very small, and a low Mach number approach is well adapted for such flows. The liquid being considered as incompressible, an adequate model must be able to take into account both a truly incompressible flow and a low Mach number flow, separated by a dynamic interface across which the physical properties of the fluid are discontinuous.

We present such a model together with a numerical method aimed at the effective and efficient computation of such two-phase flows. The model is based on the solution of the Navier-Stokes equations, and it is developed by using a one-field approach, where the liquid or the gas is indicated by a Heaviside function. The low Mach number model in the gas involves two pressures, the usual dynamic pressure and a thermodynamic pressure which is defined only in the gaseous regions and is obtained using integral relations. The numerical model uses a lagrangian front-tracking method to deal with the interface. This method has shown to be effective for complex multidimensional situations including interface merging/breakup and phase change (Tryggvason et al. (2001) or Shin et al. (2002)).

To validate our model, we present an application in a one-dimensional case where the effects of the thermodynamic pressure are significant. Comparison with a reference solution shows that the front tracking model gives accurate solutions, and is adequate for treating multidimensional application involving compressibility effects.

PHYSICAL MODEL

We consider a two-phase liquid-gas flow, the liquid phase being incompressible and the gaseous phase being compressible. The Mach number in the compressible phase is supposed to be always small. The flow can then be represented using a low Mach model as proposed by Paolucci (1986). In this model, the pressure is decomposed in two components, a thermodynamic pressure which is uniform in space, and the usual hydrodynamic pressure which is involved in incompressible flows. Let us introduce a Heaviside function $H(x,t)$, which plays the role of the characteristic function of the gaseous phase (H is equal to 1 in the gas, and 0 in the liquid phase). The function H is simply advected with the fluid velocity, and follows a transport equation :

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \vec{v} \cdot \nabla H = 0$$

The two-phase single-field model can be written, expressing the conservation of mass, momentum and energy:

$$\begin{cases} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \\ \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} + \frac{1}{\rho} \nabla \pi = \frac{1}{\rho} \nabla \cdot \tau \\ \frac{\partial T}{\partial t} + \vec{v} \cdot \nabla T = \frac{1}{\rho c_p} \nabla \cdot (k \nabla T) + \frac{1}{\rho c_p} \frac{dP}{dt} H \end{cases} \quad (1)$$

where $P(t)$ is the thermodynamic pressure, π is the hydrodynamic pressure and τ is the viscous tensor. The effect of gravity and surface tension is not included here. The gas is assumed to follow a perfect gas law:

$$P = r \rho_g T \quad (2)$$

with $r = c_p - c_v$. The liquid being considered as incompressible has a constant density ρ_l . For our two-phase model, the generalized equation of state then writes:

$$\rho = H \rho_g + (1 - H) \rho_l = H \frac{P}{rT} + (1 - H) \rho_l \quad (3)$$

The thermodynamic pressure must be calculated by using integral relations that will be derived in the

following. In equations (1), the coefficients c_p and k are discontinuous across the interface, and are obtained in the same way as in (3) from their values in the gas and in the liquid.

Using equation (3), the temperature equation in (1) can also be written in the following form, using the grouping $(1/P)(dP/dt)$ rather than dP/dt :

$$\frac{dT}{dt} = \frac{1}{\rho c_p} \nabla \cdot (k \nabla T) + \frac{\gamma - 1}{\gamma} T \frac{1}{P} \frac{dP}{dt} H \quad (4)$$

Let us now derive the integral relations for $P(t)$. To this aim, we insert (3) in the mass equation in (1) obtaining:

$$\nabla \cdot (\vec{v}) = H \left(\frac{1}{T} \frac{dT}{dt} - \frac{1}{P} \frac{dP}{dt} \right) \quad (5)$$

Let us suppose that the gaseous phase is enclosed by walls or the liquid phase (case of bubbles for example), and let us denote by $\Omega_g(t)$ its spatial extension, $\Sigma_g(t)$ the bounding surface. We then integrate (5) over $\Omega_g(t)$ to obtain:

$$\frac{1}{P} \frac{dP}{dt} = \frac{1}{\int_{\Omega_g(t)} H dx} \left(\int_{\Omega_g(t)} H \frac{1}{T} \frac{dT}{dt} dx - \int_{\Sigma_g(t)} \vec{v} \cdot \vec{n} dS \right) \quad (6)$$

In this way we calculate $(1/P)(dP/dt)$ to obtain the source term in (4). Once $(1/P)(dP/dt)$ is known, the pressure $P(t)$ can be obtained directly from a time integration, i.e.:

$$P(t + \delta t) = P(t) \cdot \exp \left(\int_t^{t+\delta t} \frac{1}{P} \frac{dP}{dt'} dt' \right) \quad (7)$$

EFFECT OF THE THERMODYNAMIC PRESSURE ON THE DYNAMICS OF THE FLOW

The model described above does not take into account the effect of thermodynamic pressure that can be encountered for example if several bubbles are enclosed in a liquid. In this case, each bubble has its own pressure, and the net effect of these pressure forces result in an acceleration of the liquid. Let us illustrate this on a simple 1D model case: a gaseous zone enclosed inside two liquid moving zones. The incompressible motion of the liquid in 1D is a uniform velocity, named $V_1(t)$ and $V_2(t)$ respectively. If we assume that the gas density ρ is uniform in space (isothermal case), the formulation of the problem in the gas reads (neglecting viscous effects):

$$\begin{cases} \frac{\partial u}{\partial x} = -\frac{\dot{\rho}}{\rho} \\ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{1}{\rho} \frac{\partial \pi}{\partial x} \end{cases} \quad (8)$$

where the notation $\dot{\rho}$ denotes the time derivative of ρ . The density can be calculated directly considering the conservation of total mass M_0 in the gaseous enclosure of instantaneous length $l(t)$, that is $\rho(t) = M_0 / l(t)$. An origin being fixed, let us denote by $l_1(t)$ and $l_2(t)$ the positions of the left and right liquid-gas interfaces respectively. One can easily show that the local velocity in the gas is given by:

$$u(x, t) = \frac{x - l_1}{l} V_2 - \frac{x - l_2}{l} V_1 \quad (9)$$

Replacing this expression in the momentum equation, one obtains the value of the pressure gradient as:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{1}{\rho} \frac{\partial \pi}{\partial x} = \frac{\ddot{l}}{l} x + \frac{\ddot{l}_2 l_2 - l_1 \ddot{l}_1}{l} \quad (10)$$

On the interfaces, this gives:

$$-\frac{1}{\rho} \frac{\partial \pi}{\partial x} = \begin{cases} \ddot{l}_1 = \dot{V}_1 & x = l_1 \\ \ddot{l}_2 = \dot{V}_2 & x = l_2 \end{cases} \quad (11)$$

The velocities being uniform inside the liquid zones, this means that the hydrodynamic pressure gradient must be uniform in the liquid in order to incorporate the thermodynamic pressures exerted by the gaseous zones enclosing the liquid. Thus we must have:

$$\frac{1}{\rho} \frac{\partial \pi}{\partial x} = \frac{1}{\rho_l} \frac{\Delta P}{L} \quad (12)$$

in each liquid zone of length L , ΔP being the thermodynamic pressure difference exerted on the liquid. This will be taken into account in the numerical model through a source term added in the momentum equations, as will be developed below.

NUMERICAL SOLUTION

The model described above must be coupled to a specific method for tracking the liquid-gas interface. Among the existing methods, we have chosen here to use the lagrangian front tracking method developed in Tryggvason (2001) and subsequent papers. This method uses a lagrangian discretization and movement of the interface. A Heaviside function, defined on the Eulerian grid, is built from the lagrangian definition of the interface. This H function is smoothed over 3 to 4 cells for numerical stability reasons. This leads to the existence of a "mixing" zone between the two fluids, where the model has no physical meaning.

The spatial discretization is based on centered finite differences for both the convection and diffusion terms. A staggered mesh is used, where hydrodynamic pressure and temperature are located at the center of the cells, while the components of the velocity are located on the faces. We have used here a first order explicit temporal discretization, but the extension to semi-implicit second order should not be a problem. A classical prediction-

projection algorithm is used to compute the velocities. In order to take into account the effect of the thermodynamic pressure, a source term is added in the prediction step of the velocity that allows the hydrodynamic pressure to reproduce the behavior established in the previous section. The predicted velocity \vec{v}^* is calculated from:

$$\frac{\vec{v}^* - \vec{v}^n}{\delta t} = -\vec{v}^n \cdot \nabla \vec{v}^n + \frac{1}{\rho} \nabla \cdot \tau^n + (1-H) \frac{1}{\rho_l} \nabla \Pi \quad (13)$$

The added source term is the last term in (13), and is the multidimensional generalization of the right hand side of equation (12). It is null in the gas, where $H=1$, and it is constant in liquid zones. The function Π is constructed such as to be defined everywhere in the spatial domain. It extends the thermodynamic pressure defined in the gaseous zones in the liquid zones where it is not defined. To construct it we impose the following conditions:

- it should be equal to the thermodynamic pressures in the gaseous zones,
- it should be harmonic in the liquid zones, in order to leave the velocity field in the liquid divergence free,
- it should verify a Neumann boundary condition on the walls.

Π can thus be interpreted as the potential in the liquid of the forces due to the thermodynamic pressures in the gaseous phases. Let us suppose that there exists N closed gaseous zones in the domain, each marked by a characteristic function H_j . The global characteristic function H is equal to the sum of the N functions H_j . We can express the above conditions through the following equation that must be verified by Π :

$$\Pi \cdot \sum_{j=1}^N H_j + (1-H) \cdot \Delta \Pi = \sum_{j=1}^N H_j P_j$$

supplemented with Neumann boundary conditions on the walls if the domain is closed. This implies that we have to solve a Helmholtz equation to calculate Π . The hydrodynamic pressure is then calculated by solving the following Poisson equation:

$$\nabla \cdot \left(\frac{1}{\rho} \nabla \pi \right) = \frac{1}{\delta t} (\nabla \cdot \vec{v}^* - \nabla \cdot \vec{v}^{n+1}) \quad (14)$$

in which $\nabla \cdot \vec{v}^{n+1}$ stands for the desired divergence of the projected velocity, which is computed using the mass conservation equation (5), after the temperature and the integral in (6) have been calculated. Once the hydrodynamic pressure is obtained, the velocity is calculated from:

$$\vec{v}^{n+1} = \vec{v}^* - \delta t \frac{1}{\rho} \nabla \pi - \delta t (1-H) \frac{1}{\rho_l} \nabla \Pi \quad (15)$$

The last term is subtracted from \vec{v}^* because the thermodynamic pressure effect is already taken into

account in the hydrodynamic pressure field, and otherwise would be taken into account twice.

To summarize, the complete algorithm reads as follows:

- Initialization
- Begin the time loop
- Solve Eq. (4) for T^{n+1} .
- Calculate H^{n+1} using the front-tracking method
- Calculate $\left((1/P)(dP/dt) \right)^{n+1}$ and P^{n+1} in each gaseous domain using \vec{v}^n , H^{n+1} and T^{n+1} in (6) and (7).
- Calculate ρ^{n+1} using (3) and update the values k , c_p .
- Calculate Π and the source term in the momentum equations.
- Calculate $\nabla \cdot \vec{v}^{n+1}$ for the Poisson equation using the mass equation (5).
- Calculate the predicted velocities \vec{v}^* from (13).
- Solve (14) for the hydrodynamic pressure π (multigrid).
- Project the velocity by (15).
- End of time loop.

For closed domains, an important point to emphasize is the compatibility relation that must be verified when processing the integration of (6) to calculate $\left((1/P)(dP/dt) \right)^{n+1}$. In this case, if we integrate (6) over the whole domain, the surface term must be zero. However, in the front-tracking method, we have pointed out the existence of a mixing zone, typically a few cells thick, inside which the velocity is only defined as an interpolation between the liquid velocity, which is divergence free, and the gas velocity which is not divergence free. Thus there is no chance that the global balance of the velocity on the interfaces be zero if the integration for each gaseous volume ends inside this mixing zone. In fact the integration must cross it and end in the liquid, or equivalently take into account all values of H which are not zero. This is a crucial point to get a correct balance of the thermodynamic pressure effects on the liquid zones.

REFERENCE ALE 1D NUMERICAL METHOD

In order to get a reference solution, we also have developed, in the 1D case, a code based on a Arbitrary Lagrangian Eulerian (ALE) method (moving mesh). In this way, the interfaces between liquid and gas are real discontinuities, and there are no errors that could be ascribed to the front tracking method and the existence of a mixing zone. Using an accurate discretization, we can consider the results given by this code as reference results. Let us emphasize that the ALE method is limited to small distortions situations in the multidimensional case, and is not adequate for treating complex multiphase flows, as opposed to the front-tracking method.

We here briefly recall the ALE method. The domains moving with time, linear transformations are used to map the physical domains to a reference mathematical domain. The spatial discretization uses a high order spectral element for each sub-domain, with order p for the temperature, density, velocity and order $p-2$ for the hydrodynamic pressure. The mapping being time

dependent, it yields additional correction terms in the governing equations to account for the mesh velocity. The time integration of the flow involves diverse time discretizations and numerical methods for the inversion of the resulting discrete operators. The complete numerical methodology is detailed elsewhere (see Duluc et al. (2008)), and we simply mention here that an iterative procedure is used at each time step in order to get converged values of the thermodynamic pressure and the temperature, velocity and density fields.

NUMERICAL RESULTS FOR A 1D PROBLEM

We consider a one-dimensional fluid system consisting of two layers of gas (air) enclosing a layer of liquid (water). The system is closed by two walls. The total length of the system is 100 μm , the length of the liquid layer is 10 μm , the latter being initially situated at the center of the system. The initial thermodynamic conditions are $P_0=101325 \text{ Pa}$, $T_0=293.15\text{K}$. At initial time, the left wall is heated to $T_w=373.15\text{K}$. The right wall is insulated. After a transient evolution, a steady state establishes where the initial positions of the liquid-gas interfaces are recovered, due to mass conservation. In the gas, the density at steady state is unchanged, $T_f = T_w$ everywhere, and $P_f=P_0 T_f/T_0=128976.37 \text{ Pa}$ following the perfect gas equation of state.

The domain is discretized using 100 grid points. The time step is equal to 10^{-8}s , due to stability limits of the explicit time discretization.

We represent in Fig.1 trajectories of the two liquid-gas interfaces. The first remark that can be done is that those trajectories are parallel (the liquid has a solid body movement), and that the initial positions are well recovered. This is a very important and demanding case to test for mass conservation for the method. A method we developed previously based on a single pressure approach (Daru et al. (2006)) revealed very serious problems with this criterion.

A logarithmic representation of the interface trajectory (Fig. 1b) reveals that in the first moments after the heating of the left wall, an oscillatory movement of the liquid zone is observed. This effect which is entirely due to compressibility of the gas was analyzed in details by Duluc et al. (2008). The corresponding thermodynamic pressure history is shown in natural (Fig. 2a) and logarithmic (Fig. 2b) scales. As the pressures in the two gaseous domains are not equal, the liquid is accelerated. In Fig. 3 is shown the fluid velocity in the whole domain, for two successive times. One can remark that the velocity is constant in the liquid, showing that the liquid behaves as a solid in this 1D case, and that compressibility effects produce a non-uniform velocity in the gas. In the first microseconds, large velocities can be attained. The hydrodynamic pressure at $t=1 \mu\text{s}$ is shown in Fig. 4. The temperature fields for several successive times is shown in Fig. 5 and reveals that after an initial transient where a piston effect can be observed in the left gaseous zone, a purely conductive regime takes place in the left gaseous zone while the temperature is nearly uniform in the right gaseous zone due to the adiabatic wall condition. The relative total mass variation in the cavity never exceeds 0.5% throughout the unsteady evolution, demonstrating good mass conservation properties of the algorithm.

Finally, in Figs. 6 and 7 we compare the results given by the front-tracking algorithm and the ALE approach, the latter being considered as the reference. It can be seen on the trajectories and the pressures history, that the results are very close (Figs. 6 and 7), although the front-tracking algorithm is only first order in time. This validates the low Mach compressible/incompressible approach in the front-tracking framework.

CONCLUSION

We have constructed a model aimed at the numerical simulation of liquid-gas flows, where compressibility effects in the gas are taken into account using a low Mach approach. The interface is treated using a front-tracking approach, which has shown to be effective in complex multidimensional situations. The model has been validated in the one-dimensional case by comparison with reference results obtained using an ALE approach. Work is currently in progress to develop multidimensional applications and to extend the model to liquid-vapor phase change problems.

NOMENCLATURE

c_p	specific heat at constant pressure J/kgK
c_v	specific heat at constant volumetric J/kgK
k	thermal conductivity W/mK
H	Heaviside function
P	thermodynamic pressure Pa
t	time s
T	temperature K
\vec{v}	velocity m/s
γ	specific heat ratio
π	hydrodynamic pressure Pa
ρ	density kg/m^3
τ	viscous tensor Pa

Subscripts

g	related to the gaseous phase
l	related to the liquid phase

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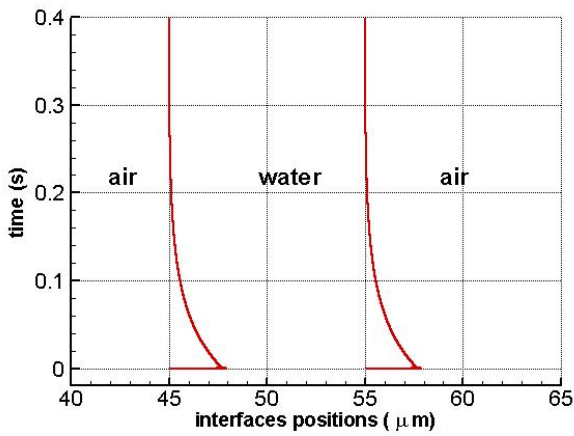


Fig. 1a Trajectories of interfaces in natural time scale

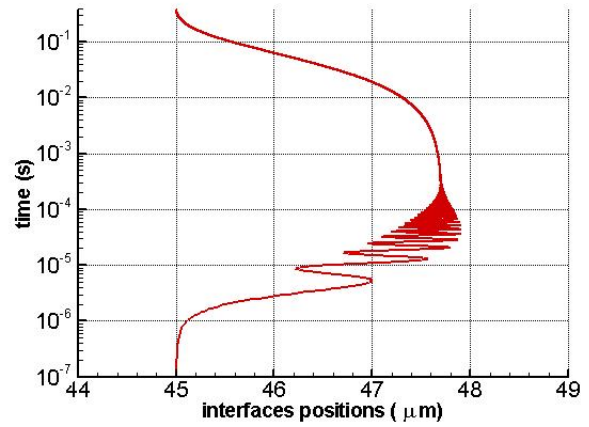


Fig. 1b Trajectories of interfaces in log time scale

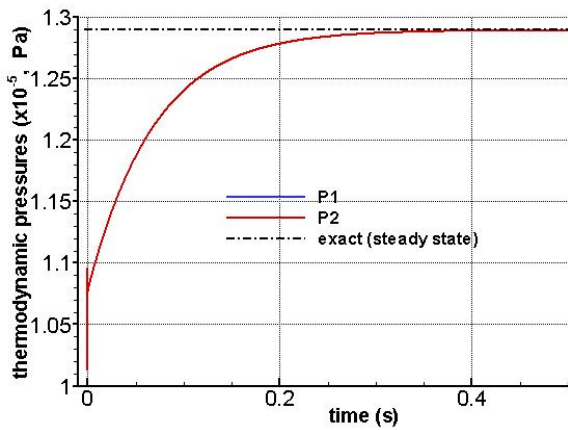


Fig. 2a Thermodynamic pressure in the gaseous domains (natural time scale)

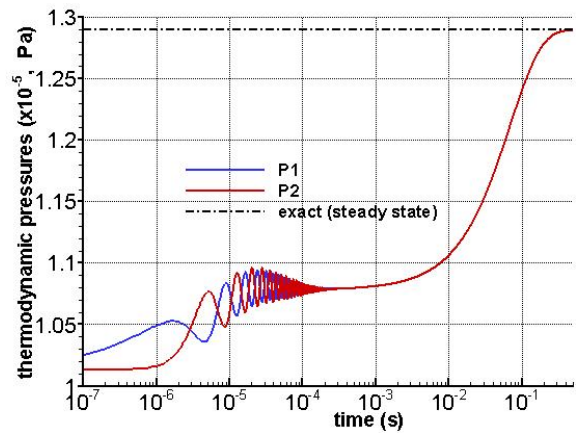


Fig. 2b Thermodynamic pressure in the gaseous domains (log time scale)

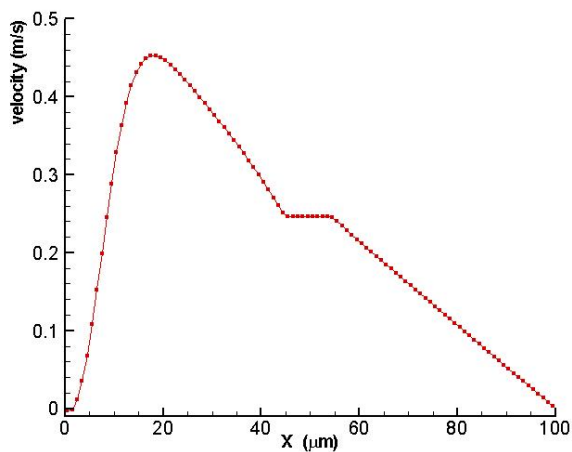


Fig. 3a Velocity field at time $t=1 \mu\text{s}$

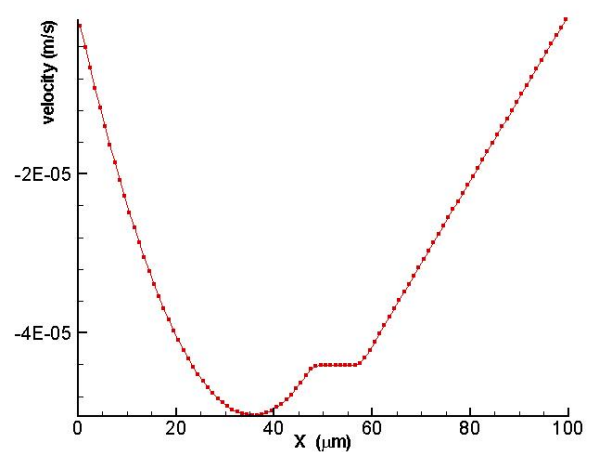


Fig. 3b Velocity field at time $t=1 \text{ ms}$

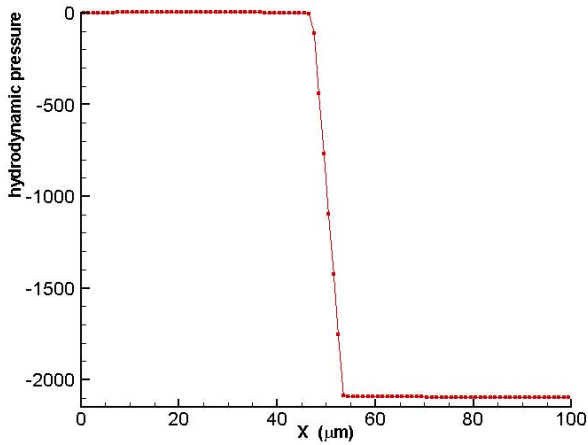


Fig. 4 Hydrodynamic pressure at time $t=1 \mu\text{s}$

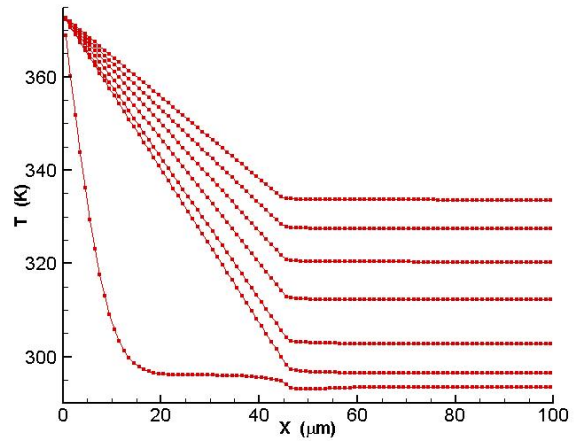


Fig. 5 Temperature field at time $t=1 \mu\text{s}$,
 $t=4, 5, 6, 7, 8, 9 \text{ ms}$

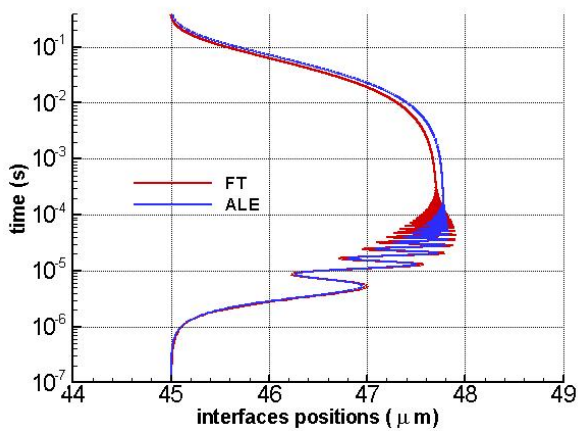


Fig. 6 Comparison of front-tracking (FT) and ALE results: left interface trajectory

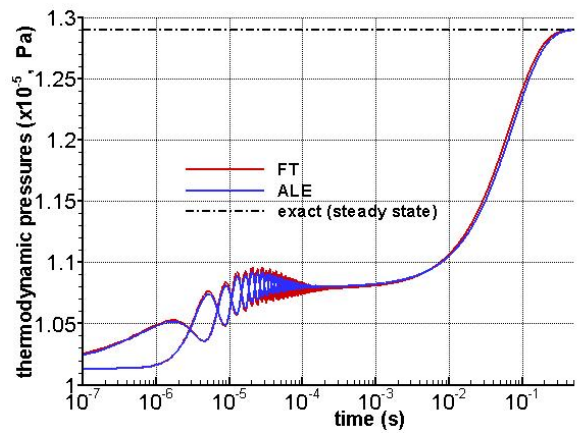


Fig. 7 Comparison of front-tracking (FT) and ALE results: time evolution of the thermodynamic pressure