THINS project: Description of the VOF based pressure algorithm and application to XT-ADS like spallation target

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Abstract

The simulation of Heavy Liquid Metal Vacuum complex interfaces with Starccm+ from CD-Adapco using the Volume of Fluid (VOF) framework requires specific care. In a first part, we describe how we managed to deal with the high density ratio and the interface smearing in the context of three different windowless spallation targets. The interface smearing is controlled with a non-conservative condensation term. The second part is dedicated to the individuation of the relevant physical process leading to the interface sharpening and its inclusion in the set of constitutive equations. The methodology used has been to re-derive the VOF equations for momentum and phase transport from the constitutive phase equations. Two candidates for sharpening are individuated: baro-diffusion and surface tension effects. Only baro-diffusion is however likely to have the required strength in the foreseen applications.

1 Introduction

This document resumes the activity performed at CRS4 in the framework of the THINS project regarding CFD simulations based on the Volume of Fluid (VoF) implementation in Starccm+ from CD-Adapco [1]. The applications primarily focus on the design of windowless spallation targets but also consider pool-like primary coolant loops of Accelerator Driven Systems (ADS). The heavy phase is a heavy liquid metal, in practice Lead-Bismuth Eutectic LBE. The light phase is either near vacuum for the spallation targets, or a neutral gas (Argon) at about atmospheric pressure. The point of view is that of a end-user of Starccm+, the primary objective being to manage to perform sound and informative simulations. The secondary objective, much more ambitious, is to enforce the coherence of the implementation with the general physico-numerical framework.

To realize the first objective, we have to recognize the limits of the VOF implementation in Starccm+. We must stress the fact that the software has about two new releases each year usually associated with improvement in robustness and liability, and with new features. In addition, we, the end-users, hopefully improve our capacity to deal with the software. This is to say that the limit of the software as seen by the end user is continuously changing in time due to software and user evolution. These limit have been investigated before and at the beginning of the project (Mars 2010) and may be partially obsolete at report time and completely obsolete a few month later.

The Starccm+ VOF implementation is globally very robust and practical. It works very satisfyingly in many cases, but we have been faced with three second order drawbacks. First, we could not stabilise any VOF simulation with a density ratio largely greater than one thousand. Second, a parasite velocity fields spontaneously develops in the light phase just above a stagnant zone of the heavy phase. Third, for flows combining both interface shear and oscillations, un-physical smearing of the interface may occur.

In the first part of the document, we describe how we have faced these drawbacks in practical applications. The methodology is quite engineeristic and pragmatic. It is not entirely satisfying from the scientific point of view.

The second part of the document is motivated by the following consideration: it is possible that the VOF limitations are not only due to difficulties in the numerical implementation, but also comes from defects in the constitutive equations at the basis of the VOF algorithm. These equations consider a priori the phases as immiscible while they cannot always be in a numerical simulation. Think for example of a case in which a small volume of gas is entrapped in a liquid and the volume is small enough to fill only partially one computational cell. It could be thus not necessarily a bad idea to inquire if we could construct the basis equations for two phases that can mix but tend to separate. The second part of the document is dedicated to such a construction.

Both parts resume a series of much more detailed documents shortly described in the third part of the document.

2 Pragmatic implementation

For the practical implementation of simulation of windowless targets, we have been faced with the following drawbacks:

1. **Density ratio** Failure to stabilize a simulation with a density ratio somewhat greater than one thousand.
2. **Stagnation flow** Parasite flow in the light phase just above a stagnant region of heavy phase.
3. **Interface smearing** Combination of oscillatory motion with shear stress may lead to unphysical interface smearing.

2.1 VOF issues

We describe hereafter how we have dealt with the VOF issues.

2.1.1 Density ratio

The windowless targets were expected to operate under near vacuum condition in the EUROTRANS framework and under very low pressure, a few Pascal, in the ESS framework. For application to the MYRRHA primary coolant loop, the cover gas, possibly Argon, is foreseen slightly below atmospheric pressure. In all cases, the foreseen coolant is LBE with a density above ten thousand. And in all cases, the density of the light phase is order one or quite below. So, the density ratio is critically out of the range of stability of VOF simulation that we found out to be slightly over one thousand, typical of the water/atmospheric air density ratio. the density ratio issue has been by-passed by either lowering the LBE density by a factor of ten or increasing the light phase density to about ten. As our primary interest is in the LBE flow, and to have the correct pressure gradient there, the preferred method has been to modify the light phase density.

In the case of very low pressure light phase, the treatment of the light phase as incompressible becomes very questionable. We believe that the error introduced by the wrong light phase incompressibility is much more critical than the error induced by the increase of density, even by several orders of magnitude. What is important is that the light phase remains light in confront with the heavy phase. Willingly, a ratio of one hundred should be far enough to capture the main relevant (heavy phase) flow features. We have however usually kept the one thousand ratio.

2.1.2 Stagnation flow

Parasite flows develop in the light phase just above a stagnant region of heavy phase. We suspect that these parasite flows are a precursor of the complete flow instability encountered for density ratios higher than one thousand.

As we have already renounced to have meaningful information on the light phase behaviour with the density ratio issue, no specific counter-measure is taken. The parasite flows however may alter the quality of some illustrative plots.

2.1.3 Interface smearing

This issue is the most serious of the list. It is not commonly encountered. In effect, the star-ccm+ VOF implementation is very resistant to flows showing a strong shear at the interface. It

also propagates very well a liquid front. We have encountered interface smearing only in flows subject to oscillatory motion, thus involving interface acceleration, together with shear stress. The problem has been encountered twice in the same simulation. In one region of relatively slow motion the surface oscillation was combined with a convergent flow on the surface. The other region was stressed combining a pulsed behaviour with a swirling downcoming free-surface. The smearing of the interface could be put in evidence by plotting some transverse section of the concentration and by making a double localization of the surface using two different iso-surface of the volume fraction, one with value 0.1 and the other with value 0.9. In both cases, the interface smearing was due to the fact that the portion of stressed smearing interface was trapped in loco and not evacuated by convection out of the simulation domain.

The issue has been solved by implementing a source term, which is in fact a sink term, in the light phase volume fraction transport equation. As already mentioned, we have renounced to any pretension on the physical relevance of the light phase flow. Therefore, such a source term is only altering something already wrong. If the alteration reduces the negative impact of the light phase on the heavy one, we are happy with it.

The sink term is localized at the interface. As the interface most simple localisation is the region where the product of the volume fraction is non zero, the sink term has been made proportional to this product. The coefficient of proportionality, which is the inverse of a characteristic time has been set so as to induce a small current towards the interface, whose speed is one order less than the characteristic speed of the heavy phase when the interface is reasonably sharp. The advantage of such a sink term is that it scales proportionally to the interface width and thus cancels in theory when the interface is sharp.

Several other terms have been tested, increasing the polynomial or the derivation order, but always leading to a lowered efficiency. The more common defect being not allowing to correctly clean the light phase from small heavy phase residuals. In the end, the simplest term resulted to be the better one.

The introduction of this sink term allowed us to investigate VOF flows with a reasonable confidence when the heavy phase is in a closed loop.

The introduction of the sink term is not likely to have a good or neutral effect of the heavy phase flow accuracy in all configurations. In effect, it requires that the consumed light phase is replaced naturally by fresh new light phase. This is possible only when all the connected parts of the light phase are in contact with a boundary of the simulation domain capable to deliver the new fresh light phase. A careful examination must be performed on a case by case basis.

The overall intensity of the sink term is not known a priori and is likely to evolve in time. A classical inlet boundary condition is therefore not suited in this case. A pressure outlet used to give at least a code warning and numerical countermeasure when measuring a tentative inlet flow. Pressure outlets also tend to be unstable when they are very large. One possible solution is to add a light phase source term close to the outlet pressure boundary with an intensity quite larger than the sink term (it can be adjusted dynamically). The other solution we could find, which resulted very convenient, is to set a stagnation inlet pressure. This is a type of boundary condition thought for compressible flows but it works perfectly for our purpose. The stagnation inlet is complemented with a relatively small sink term so that the condition is in fact an inlet condition independently of the size of the interface and even if the contracting source term is turned off.

3 Other simulation issues

Running a simulation in the VOF framework becomes routine only after a long history of failures. We present here the main procedures we have been progressively led to undergo such simulations. Knowing that VOF simulations are necessarily transient even if one expect a final stationary behaviour, we consider now two critical features: the initial condition and the reduction of the transient behaviour to the nominal condition behaviour.

3.1 Initial conditions

Contrarily to many single phase simulations, VOF simulations depend largely on the initial condition, even for asymptotic large times. This is particularly true for our applications in which we consider

a closed loop of LBE. The initial LBE mass will be conserved during the simulation, unless a specific source term is added.

As soon as the simulation is not completely trivial, the asymptotic position of LBE is not necessarily known and the asymptotic velocity field becomes quite articulated. We have found more easy to begin the simulation with a stagnant flow. The flow is then progressively accelerated to reach the asymptotic pattern. The initial stagnant configuration need not be stable. It can be set so as to reduce the transient time needed to reach the asymptotic behaviour.

What is very critical is the initial pressure setting. The initial pressure field is generally not known, unless the initial configuration is stable. Mainly when the initial interface is everywhere at the same level and at rest, then the initial pressure field is the static pressure field. Even in this case, there are slight but noticeable differences between the theoretical initial pressure field and the discretized pressure field. If this difference is loaded on the light phase at the interface, then the simulation diverges on the spot.

The solution we have found out is to start the simulation at rest but not necessarily in static equilibrium, using at start some extremely small time steps with a relatively large number of iterations. The pressure has thus many iteration to settle and enforce the incompressibility constraint but the acceleration induced on the flow is integrated on a very small time laps and even if the acceleration is huge, the increase in velocity is small. With a large enough number of iteration for the first time steps, the pressure has settled before that the flow has been disrupted and the simulation diverged.

3.2 Transient acceleration

According to the CFL condition, the limitation on the time step is very stringent. As we start from the flow at rest, the route to the asymptotic nominal condition takes some physical time. Note that for many applications, the nominal condition is not the aim of the simulation but is the start of the interesting part of the simulation. This is particularly true when investigating incidental or accidental scenarios as well as for example a controlled shut-down procedure. The fact is that we have usually not the necessary material time to reach the nominal condition respecting the rules of the art. The problem is not solvable through a huge increase of computational power, because the simulations are run in parallel on several CPUs and the speed up decreases very fast under a certain number of computational cells by CPU. Here, the small time step has been the main controlling parameter. To limit the computational time, it is therefore necessary to increase largely the time step and reduce at the maximum the number of iteration by time-step. Making exception with the very first time steps. The time step increase is limited only by the stability of the simulation. However, two particular damages occur. First, the interface is smeared. Second, the overall heavy phase is no more perfectly conserved. The interface smearing can be controlled by the the sink term previously described. The mass loss has to be dealt with, specially in pool of loop configuration. Otherwise, the mass loss is compensated by the inlet outlet balance. What we have done has been to monitor the LBE total mass and inserted a source term in a region remote from the free-surface proportional to the deviation of the total mass. The source term is normally very small because the total mass varies very little. The characteristic time of return is problem dependant and could be set about one second. It is also very convenient to use to adapt the total mass to the required behaviour when the "right" value is not known precisely. This has been particularly true when working on an alternative windowless target for XT-ADS.

4 VOF extension

All the procedures presented allowed to realize many VOF simulations giving useful insight on the heavy phase flow. The main limitation is that almost nothing can be said on the light phase flow. However, we would be interested also in the light phase flow. Of particular relevance would be to represent evaporation processes. Even in absence of those, a control of the cover gas temperature would be welcome. This is clearly impossible using the former methodology because the light phase is not conserved.

Writing a conservative sharpening procedure results however much more delicate than just adding a sink term. To be conservative, the corrective terms are likely to be the divergence of some flux

cancelling where the fluid is completely separated. In turn, the end-user has no access to add arbitrary fluxes in the Starccm+ equations. Only source term can be added, but a flux divergence treated as a source terms does not obey any discrete form of the divergence theorem due to a larger method of discretisation. A flux divergence is treated numerically in a very specific way. And so, it is impossible for a end-user to implement a conservative sharpening method. An alternative is to convince the CD-Adapco developers to give access to flux divergence terms or make themselves the implementation. It is necessary to provide them the flux to be implemented, their utility and their theoretical justification. What we do in the following is thus the theoretical derivation of the necessary flux to be implemented.

The methodology has been the following:

- Postulate single phase equations consistent with the global momentum equation.
- Identify the effects of the forces applied to the single phase equations.
- Select the forces likely to have a sharpening effect.
- Relate the forces to the corrective flux in the phase transport equations.

4.1 Notations

We are dealing with two phases, possibly mixing. One is named A and the second B. While not necessary we will think of A as the heavy phase. The physical quantities associated with A will have subscript a except the volume fraction which will be exactly a. Same thing for B. The global physical quantities will not have any subscript. The principal notations/definitions are:

- **Density**: $\rho = a\rho_a + b\rho_b$.
- **Mass velocity**: $u = \rho^{-1}(a\rho_a u_a + b\rho_b u_b)$.
- **Volume velocity**: $v = au_a + b_{ub}$.
- **Shared pressure**: P.
- **Extra-stress tensor**: τ.
- **Gravity acceleration**: g.
- **Generic force**: $F = F_a + F_b$.
- **Generic residual force**: $F_0 = \rho^{-1}(b\rho_b F_a - a\rho_a F_b)$
- **Correction flux**: $\phi = -ab(u_b - u_a)$.

4.2 Constraints

The physical constraints are the mass conservation of both phases , the incompressibility of the phases, and the obligation for the mixture to fill the space.

- ρ_a and ρ_b are constant in space and time.
- $\partial_t a\rho_a + \nabla \cdot a\rho_a u_a = 0$.
- $\partial_t b\rho_b + \nabla \cdot b\rho_b u_b = 0$.
- $a + b = 1$.

The global incompressibility of the mixture is easily deduced, but applies to the volume velocity:

$$\nabla \cdot v = 0.$$

The "safety" constraint is to not alter the global momentum equation as given by Landau. We slightly relax this constraint in the sense that the surface tension force can be somewhat generalized to a generic force.

$$\partial_t \rho u + \nabla \cdot \rho u u + \nabla P + \nabla \cdot \tau = \rho g + F$$

4.3 Phase momentum equations

We postulate the general form of conserved material properties X_a of phase A from consideration on an arbitrary fixed control volume, as:

$$\partial_t a\rho_a X_a + \nabla \cdot a\rho_a u X_a + \nabla \cdot \Phi = I_a + \dot{S}_a$$

where

- $a\rho_a u X_a$ is the convection flux, the approximated main flux based on the global mass velocity.
- Φ is the corrective flux to equilibrate the balance.
- I_a is the term of exchange of $a\rho_a X_a$ with the other phase
- $\dot{S}_a$ is the source of $a\rho_a X_a$.

The general equation is then specialized by taking $X_a = u_a$:

$$\partial_t a\rho_a u_a + \nabla \cdot a\rho_a u u_a + \nabla \cdot a[P + P_0(t)I + \tau] = I_a + a\rho_a g + F'_a$$

In the incompressible framework, the pressure is defined up to a constant. However, this constant is only constant in space but not necessarily in time. We will need to precise this time dependence, motivating the appearance of P_0.

To separate the effects, we extract from the correction flux the terms depending on ∇a and group them the with the last term F'_a to give F_a.

$$\partial_t a\rho_a u_a + \nabla \cdot a\rho_a u u_a + a\nabla P + a\nabla \cdot \tau = I_a + a\rho_a g + F_a$$

and for phase B:

$$\partial_t b\rho_b u_b + \nabla \cdot b\rho_b u u_b + b\nabla P + b\nabla \cdot \tau = I_b + b\rho_b g + F_b.$$

These equations clearly sum to give back the global momentum equation on the condition that $I_a + I_b = 0$ normally satisfied for exchange terms.

4.4 Phase potential terms

There are two terms in the phase momentum equation that can be interpreted in terms forces derived from a potential: $a\rho_a g$ and $a\nabla P$. We would like a third one, namely F_a to share the same property.

The potentials from which a force is derived are found by solving $\partial_t E_a = -\int_\Omega F_a u_a$ where the domain of integration Ω is in fact the periodic cube to allow part integration without boundary terms. The equation can be solved by using the phase transport equation. The formula is based on the hypothesis that Newton'law can be applied and that for an isolated phase driven only by this potential, the total energy of the system is preserved, and thus the time variation of the kinetic energy plus the potential energy is zero.

A hidden hypothesis is the additivity of Newton's law to an arbitrary number of particles. The acceleration of a group of particles is not in general equal to the acceleration of the single particles. A noticeable exception is the gravity force which accelerates the particles independently of their mass. With the incompressibility constraint, the separate phase treatment and the constant phase density, we place ourself in a similar specific case.

4.4.1 Gravity potential

The gravity potential of phase A associated to $a\rho_a g$ is obviously found to be $E_a = \int_\Omega a|g|z$ where z is the vertical axis.

4.4.2 Pressure potential

The time varying pressure potential associated to $a\nabla P$, is found to be $E_a = \int_\Omega a[P + P_0(t)]$ with the time dependant part defined as $P_0(t) = -(\int_\Omega a)^{-1} \int^t (\int_\Omega a\partial_t P)$.

4.4.3 Diffusion potential

A generic force pair in the phase momentum equation of the form $F_a = \mathcal{F}\nabla a$ and $F_b = \mathcal{F}\nabla b$ identically cancels in the global momentum equation. We have however included the term $-P\nabla a$ in F_a. For a perfect gas, this term is equivalent to $-(nkT)\nabla a$, with the advantage of this last term to have (nkT) constant for an isothermal flow with a volumetric number density n constant. For such a force, clearly associated to the phase diffusion, the potential would be $E_a = \int_\Omega (nkT) a ln a$.

4.4.4 Surface tension potential

Taking $E = \int_\Omega \sigma|\nabla a|$, split as $E_a = \int_\Omega \sigma b|\nabla a|$ and $E_b = \int_\Omega \sigma a|\nabla b|$, we obtain the Landau surface tension force $F = -\sigma(\nabla \cdot n)\nabla a$, with the normal n defined as $n = |\nabla a|^{-1}\nabla a$ however with the phase forces

$$F_a = \sigma[\nabla(ab\nabla \cdot n) - b\nabla \cdot n\nabla a]$$

$$F_b = \sigma[-\nabla(ab\nabla \cdot n) - a\nabla \cdot n\nabla a]$$

4.4.5 Cahn-Hilliard potential

With the Cann-Hilliard potential $E = \int_\Omega 3\sigma(\delta|\nabla a|^2 + \delta^{-1}a^2b^2)$ and charging all the potential on the heavy phase, we have $F_a = 6\sigma a\nabla[\delta\Delta a - \delta^{-1}ab(b-a)]$.

4.4.6 Surface tension potential (missing part)

The surface tension potential can be completed with a contracting part $E = \int_\Omega \sigma\delta^{-1}ab$, which is identically zero in the derivation from Landau in

which the phases are completely separated. Splitting the energy as $E_a = \int_\Omega \frac{\sigma}{3\delta} ab(1+b)$ and $E_b = \int_\Omega \frac{\sigma}{3\delta} ab(1+a)$, we have:

$$F_a = \sigma\delta^{-1} ab\nabla a.$$

4.5 Exchange term

The exchange term is usually written in symmetrical form and is given for phase A as: $I_a = Rab(u_b - u_a)$. This is the simplest consistent formula. The resistance coefficient R depends mainly on the phases mass fraction and on some reduced frequency of collision. The exchange term can be build by looking at the momentum exchanged during a binary collision at the phases mean velocity and at the collision frequency. The modelling performed here is rather approximative. The coefficient R is usually taken independent of the volume fraction and is built on the assumption that the concentration gradient is small. It is therefore perfectly possible to assume a saturation effect for strong concentration gradients and take R in a form such as $R = R_0(1+|\delta\nabla a|^2)$. Such a form will prove to be convenient later on.

A lot of work can be done on R, leading to quite different expressions. If we look at the Eulerian two-phase flows, in the turbulent regime R becomes proportional to $|u_a - u_b|$. A lot of work can be thus done on R, leading to quite different expressions, according to the case under study or to a more complex expression if we manage to capture together the different local configurations.

4.6 Dynamic equilibrium assumption

4.6.1 Force splitting

Considering a force pair, we want to split each term in one part contributing to the acceleration of the whole mixture and one residual part. We have already two extreme situations: the gravity which entirely contributes to the global mixture movement from one side, and the diffusion force having no effect on the mixture acceleration, from the other side. The splitting is the following:

$$F_a = \frac{a\rho_a}{\rho} F + F_0$$
$$F_b = \frac{b\rho_b}{\rho} F - F_0$$

giving the residual part F_0 as:

$$F_0 = \frac{b\rho_b}{F}_a - \frac{a\rho_a}{\rho} F_b.$$

We have:

- **Gravity**: $F_0 = 0$
- **Pressure**: $F_0 = \frac{ab(\rho_a - \rho_b)}{\rho}\nabla P$
- **Diffusion**: $F_0 = -(nkT)\nabla a$
- **Surface tension**: $F_0 = \frac{ab}{\rho}\nabla(\rho_\nabla \cdot n)$
- **Cahn-Hilliard**: $F_0 = 6\sigma ab\nabla[\delta\Delta a - \delta^{-1} ab(b-a)]$
- **Surface tension missing**: $F_0 = \sigma\delta^{-1} ab\nabla a$.

4.6.2 Equilibrium assumption

Our equilibrium assumption is the sum of the force residual part F_0 of phase A is equal to the momentum exchange received by phase B. That is:

$$F_0 = I_b.$$

4.7 Phase transport equation

The equilibrium assumption completely determines the correction flux in the phase transport equation. In effect, the phase A transport equation written in term of the mass velocity is:

$$\partial_t a\rho_a + \nabla \cdot a\rho_a u + \nabla \cdot \frac{\rho_a\rho_b}{\rho}\phi = 0$$

with ϕ the correction flux defined as $\phi = -ab(u_b - u_a)$.

In terms of the volume velocity, the equation reduces to:

$$\partial_t a + \nabla \cdot av + \nabla \cdot \phi = 0,$$

justifying the name given to ϕ.

As $I_b = R\phi$, from the equilibrium assumption we have:

$$\phi = R^{-1} F_0$$

where F_0 stands for all the residual forces one wants to consider.

Two forces are of particular interest for the VOF simulations. The first is the pressure force, responsible for the baro-diffusion. The second is the surface tension contracting part (the missing part).

The baro-diffusion is contracting only when the pressure gradient and the density gradient have a positive scalar product. It stabilizes a stratified flow when the heavy phase is under the light phase. The contracting part of the surface tension is more likely to have small scale effects, working locally at gathering low volume fractions in small bubbles or droplets.

In the main foreseen applications, the mesh scale is order a few centimetres, and surface tension direct effects should be discarded. For an application with the mesh cell of order one millimetre, the surface tension contracting term is likely to play a decisive role in the phase transport equation. The diffusive term, describing a flux towards the regions of greater curvature, tangentially to the interface, can still be neglected. If the contracting term is used, however, the gradient correction of the resistance coefficient R must also be used. Otherwise, as the phase force becomes unbounded when the interface becomes very thin. the drift velocity $u_b - u_a$ would also become unbounded.

The diffusive force has always an intensity higher than the other forces when the concentration becomes very low. To allow a complete separation of the phase (even with a non-zero width), it is therefore compulsory to avoid the corresponding flux in the transport equation. This is already clear in the present VOF implementation.

4.8 Incompressibility constraint

The incompressibility constraint $\nabla \cdot v = 0$ applies on the volume fraction velocity. As the momentum equation is written in terms of the mass fraction velocity, we must enforce the consistency of the system by writing also the incompressibility constraint in terms of the mass velocity. Simple algebraic manipulation gives:

$$u = v + \frac{\rho_a - \rho_b}{\rho} ab(u_a - u_b) = \frac{\rho_a - \rho_b}{\rho}\phi$$

so that the equilibrium assumption allows to write the incompressibility constraint under the form:

$$\nabla \cdot u = \nabla \cdot \frac{\rho_a - \rho_b}{R\rho}\phi,$$

this last equation completing our construction.

4.9 Equations for large pool reactors

For large pool reactors, such as MYRRHA, the foreseen discretisation will be in the centimetre range, thus not allowing to capture surface tension effects. The system of equations to be solve resumes to:

$$\begin{aligned}
\partial_t \rho u &+ \nabla \cdot \rho u u + \nabla P + \nabla \cdot \tau = \rho g \\
\partial_t a\rho_a &+ \nabla \cdot a\rho_a u + \nabla \cdot \frac{\rho_a \rho_b (\rho_a - \rho_b)}{R\rho^2} ab \nabla P = 0 \\
\nabla \cdot u &= \nabla \cdot \frac{(\rho_a - \rho_b)^2}{R\rho^2} ab \nabla P
\end{aligned}$$

It is equivalent to a system of 5 scalar equations in the fundamental variable set (u, a, P). The remaining variables b and ρ are found by elementary algebraic relations.

There are two critical differences with the VOF equations: first a correction flux in the phase transport equation and second, a correction in the velocity constraint. As these corrections are strongly related, both must be considered otherwise the consistency is lost. However, as stated before, there is a large space for modelling the coefficient R, also with the objective to stabilize the behaviour of the equations.

5 Associated documentation

The material presented here is extracted from a series of CRS4 internal reports which are shortly resumed here.

In [2], we study the free-fall version of the MYRRHA spallation target. Simulations are 2D or with a small slice in the third direction. The non-conservative sharpening algorithm is first used here. A free fall flow is obtained, but it has been impossible to manage to stabilize the reattachment region. In absence of reattachment region, that is when the LBE jet directly exits through a pressure boundary, the Starccm+ (version 4) works perfectly by itself. It was concluded that the reattachment region could be investigated only with full 3D simulations.

In [3], we evaluate a CRS4 windowless spallation target design occupying three fuel assemblies and inspired from the channel target developed for PDS-XADS. It is here that we critically encounter the limitations of the starccm+ algorithm. The emphasis is however on the consistency of the design.

In [4], we resume the first two documents and try to rationalize on the methodology used or to be used. This document is the main source for the first part of the current document.

In [5], we describe a proposal for a windowless spallation target for the future European Spallation Source (ESS). It is a direct application of the knowledge just gained on the VOF free-surface simulations.

In [6], we make an attempt to develop a comprehensive representation of two components incompressible Newtonian flows. It has been the source of the second part of the document but is much more exhaustive, mainly with regards to completely separated flows and with surface tension related features.

6 Conclusion

The VOF algorithm in Starccm+ allows to treat directly many practical situations. The range of applications can be somewhat extended by using the methodology described in the first part of the document, with direct access to the end-user.

To go further on the range of applications, we think that part of the problem lies in the constitutive equations at the bases of the VOF formulation. In this paper, we have proposed an extension of these constitutive equations to fluids that are allowed to partially mix but spontaneously tend to separate under a pressure gradient. We believe this extension to be consistent and potentially useful. There is a great distance between a mathematical formulation and its sound numerical implementation. We hope that the material presented here will convince the developers to undertake such an implementation.

7 References

The main theoretical references are found in [6]

References

[1] CD-adapco website, http://www.cd-adapco.com/ (Last access February 2012)

[2] V. Moreau, Free fall 2D+ simulation with starccmV4, CRS4 technical report CRS4-TEC-REP-10/55 http://publications.crs4.it/pubdocs/2010/MO10i/

[3] V. Moreau, Feasibility study of a CRS4 alterative spallation target for FASTEF, CRS4 technical report CRS4-TEC-REP-10/56 http://publications.crs4.it/pubdocs/2010/MO10e/

[4] V. Moreau, Free surface simulation with starccmV4 Framework and preliminary simulations resume, CRS4 internal report CRS4-TEC-REP-2010VM03 http://publications.crs4.it/pubdocs/2010/Mor10/

[5] V. Moreau, A CRS4 spallation Target for ESS Simulations with starccm+V5.0, CRS4 technical report CRS4-TEC-REP-10/57 http://publications.crs4.it/pubdocs/2010/MO10h/

[6] V. Moreau, On the representation of incompressible Newtonian free-surface CFD flows, CRS4 technical report CRS4-TEC-REP-2012VM01 http://publications.crs4.it/pubdocs/2012/Mor12/