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Sardinia Autonomous Region

# 1st THINS Cluster Workshop: CFD cluster

Basic set of equations for high density ratio free surface flow in the VOF framework

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## Application Target

- Windowless Spallation target: HLM/Near Vacuum interface
- MYRRHA primary loop: LBE/cover Gas ( $\sim 1\text{Bar}$ )

## Tool

- Starccm+ Volume of Fluid (VOF) Framework
- Navier-Stokes Equation (NSE) for incompressible fluid

## Criticalities

- Very high density ratio: numerical instability
- Highly stressed transient flows: interface smearing
- Stagnant interface: light phase spurious flow
- Computational power: free-surface not main objective of simulation

## Issue

- Immiscibility of the phases is set a priori in the equations: equations are projected onto the reduced functional space.
- VOF numerical flows are partially mixed at least on a one cell interface basis: validity of the projection is therefore questionable.

## Attack angle

- Check/re-derive equations for mixed fluids
- Start from the separate single phase equations

## Constraints

- Must give back NSE equations
- Must be resistant to classical examples
- Must clarify relation between force and diffusive flux
- Phases must tend spontaneously to separate

## Many variables

- Phase A (heavy) uses subscript a: volume fraction  $a$ , density  $\rho_a$ , velocity  $u_a$ .
- Phase B (light) uses subscript b: volume fraction  $b$ , density  $\rho_b$ , velocity  $u_b$ .
- Derived quantities:
  - density  $\rho = a\rho_a + b\rho_b$ ,
  - volume fraction velocity  $v = au_a + bu_b$ ,
  - mass fraction velocity  $u = \rho^{-1}(a\rho_a u_a + b\rho_b u_b)$
- Pressure (shared):  $P$ .

## Two valid candidates for the global velocity

Their difference is related to the phase variables:

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

no difference when both densities are equal.

## Inconsistent set of primary equations

- Momentum:  $\partial_t(\rho u) + \nabla \cdot (\rho uu) + \nabla P + \nabla \cdot \tau = \rho g + F$
- Equation of State (EoS), incompressibility constraint:  $\nabla \cdot v = 0$
- Phase A mass conservation:  $\partial_t(\rho_a a) + \nabla \cdot (a \rho_a u_a) = 0$
- Phase B mass conservation:  $\partial_t(\rho_b b) + \nabla \cdot (b \rho_b u_b) = 0$

## Rewriting of mass/volume conservation

- Phase A mass conservation:  $\partial_t(\rho_a a) + \nabla \cdot a \rho_a u - \nabla \cdot \frac{\rho_a \rho_b}{\rho} ab(u_b - u_a) = 0$
- Phase A volume conservation:  $\partial_t a + \nabla \cdot av - \nabla \cdot ab(u_b - u_a) = 0$

## Closure of the system

The system of equations for  $(u, v, a, P)$  is closed and consistent if we decide to model  $u_b - u_a$  in terms of the other variables and parameters.

# Classical closure: Fick's law

## Closure

$\phi_a = ab(u_a - u_b) = -D\nabla a$  where  $D$  is the diffusion coefficient  $m^2s^{-1}$ , gives simplest linear equation in  $a$ .

## Closed system under Fick's law closure

- Momentum:  $\partial_t(\rho u) + \nabla \cdot (\rho uu) + \nabla P + \nabla \cdot \tau = \rho g + F$
- Equation of State (EoS), incompressibility constraint:  $\nabla \cdot v = 0$
- Phase A volume conservation:  $\partial_t a + \nabla \cdot av - \nabla \cdot D\nabla a = 0$
- Velocity difference:  $u - v = \frac{\rho_b - \rho_a}{\rho} D\nabla \cdot a$

## Note

- In terms of mass fraction  $\tilde{a}$  defined by  $\rho\tilde{a} = \rho_a a$  we retrieve the classical diffusion equation (with  $u$ ):  $\partial_t \rho\tilde{a} + \nabla \rho\tilde{a}u - \nabla \cdot \rho D\nabla \tilde{a} = 0$
- When  $D = 0$  we have  $u = v$  and we retrieve the VOF implementation in Starccm+

## Cahn-Hilliard and Allen-Cahn

- Cahn-Hilliard:  $\phi_a = ab(u_a - u_b) = \alpha \nabla \Delta a - \beta \nabla ab(b - a)$
- Allen-Cahn:  $\nabla \cdot \phi_a = -\nabla \cdot \alpha \nabla a + \beta ab(b - a) + \varepsilon(t)$

related to small scale phase separation process (linked to surface tension) with negligible apparent velocity ( $v = 0$ ).

## Baro-diffusion

$$\phi_a = ab(u_a - u_b) = -D \nabla a + \gamma (\rho_a - \rho_b) \frac{ab}{\rho} \nabla P$$

related to gas separation process for which there is no surface tension

## Immiscible fluids

$$\phi_a = ab(u_a - u_b) = 0$$

because  $ab = 0$

# Postulated phase momentum equation

## General form of "all" conservation equations

from a balance over an arbitrary control volume of a property  $X_a$  of phase A

$$\partial_t \rho_a X + \nabla \cdot u \rho_a X_a + \nabla \cdot \Phi_a = S_a + I_a$$

Where  $S_a$  is the source of  $X_a$  and  $I_a$  is a term of exchange.

- $\nabla \cdot \rho_a u X_a$  "approximate" convective flux (main)
- $\nabla \cdot \Phi_a$  corrective flux (deviation)
- $S_a$  is the source of  $\rho_a X_a$  (may be more than one)
- $I_a$  is a term of exchange with the other phase

## Important notes

- The velocity used is the mass fraction velocity  $u$
- The term  $\nabla \cdot \Phi_a$  is the most strongly modelled



## Phase momentum equation: $X = au_a$ and $X = bu_b$

$$\partial_t a \rho_a u_a + \nabla \cdot a \rho_a u u_a + \nabla \cdot a ([P + P_0]I + \tau) = a \rho_a g + F'_a + I_a$$

$$\partial_t b \rho_b u_b + \nabla \cdot b \rho_b u u_b + \nabla \cdot b ([P + P_0]I + \tau) = b \rho_b g + F'_b + I_b$$

Where  $g$  is the gravity acceleration,  $P_0$  is the time dependant pressure constant (in space),  $I_d$  the identity matrix, while  $F'_a$  and  $F'_b$  are (partially) responsible for diffusion or phase separation and surface tension effects. Summing the two phase momentum equations gives back the classical momentum NSE under the conditions:

- $I_a + I_b = 0$  as we expect from exchange terms
- $F'_a + F'_b = F$

## Splitting of the corrective flux

$$\nabla \cdot a([P + P_0]I + \tau) = a\nabla P + (P + P_0)\nabla a + \tau\nabla a + a\nabla \cdot \tau$$

We can recognize the pressure force in the first term. The second and third terms are related to diffusion and are therefore coupled with  $F'_a$ . Taking  $F_a = F'_a - (P + P_0)\nabla a - \tau\nabla a$ , we have our almost final phase momentum equations:

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

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

with

- $I_a + I_b = 0$  as we expect from exchange terms
- $F_a + F_b = F$

## Representation

given a potential energy  $E_a$  of phase A, the corresponding force density  $f_a$  to be put in the phase A momentum equation is found by solving

$$\partial_t E_a = - \int_{\Omega} f_a u_a$$

it is just stating that potential plus kinetic energy is conserved and applying Newton's law to all the "particules" of phase A. This is acceptable because all particules have the same weight, otherwise an error is introduced.

## Remark

In the Cahn-Hilliard framework, the chemical potential is referred to the entire system. By splitting the potential between the phases, we slightly increase the level of description, allowing to derive the force in exact math. More precisely, we do not need any more to invoke any Lyapunov functional.

# Important examples

## Gravitational potential

with  $E_a = \int_{\Omega} a \rho_a |g| z$ , we have:  $f_a = a \rho_a g$

## Partial pressure

with  $E_a = \int_{\Omega} a(P + P_0)$ ,  $V_a = \int_{\Omega} a$  and  $P_0 = V_a^{-1} \int^t \int_{\Omega} a \partial_t P$ ,  
we have:  $f_a = -a \nabla P$  associated to baro-diffusion

## "Thermal" pressure

with  $E_a = \int_{\Omega} (nkT) a \ln a$ , where  $T$  is the constant temperature,  
we have:  $f_a = -(nkT) \nabla a$ , a good candidate for diffusion effects

## Generic

- $E_a = \int_{\Omega} H(a)$  then  $F_a = -a \nabla h$  with  $H' = h$
- $E_a = \int_{\Omega} G(|\nabla H(a)|)$  then  $F_a = a \nabla [h \nabla \cdot (gn)]$  with  $n = \frac{\nabla H(a)}{|\nabla H(a)|}$ ,  $G' = g$

# Surface tension related terms

## Landau surface tension

with  $E_a = \int_{\Omega} \sigma b |\nabla a|$ ,  $E_b = \int_{\Omega} \sigma a |\nabla b|$  and  $n = |\nabla a|^{-1} \nabla a$ ,

we have:  $f_a = \sigma a \nabla (b \nabla \cdot n)$  and  $f_b = -\sigma b \nabla (a \nabla \cdot n)$

$$E = E_a + E_b = \int_{\Omega} \sigma |\nabla a|$$

$$f = f_a + f_b = -\sigma \nabla \cdot n \nabla a$$

## Cahn-Hilliard diffusive

with  $E_a = \int_{\Omega} \frac{1}{2} \alpha |\nabla a|^2$  and  $E_b = 0$ ,

we have:  $f_a = \sigma a \nabla \Delta a = -\alpha \Delta a \nabla a + \alpha \nabla (a \Delta a)$ .

## Cahn-Hilliard contracting

with  $E_a = \frac{1}{2} \beta \int_{\Omega} a^2 b^2$  and  $E_b = 0$ ,

we have:  $f_a = -\beta a \nabla ab (b - a)$ .

## Remark

Forces are similar but not proportional to the Cahn-Hilliard fluxes.

## First modelling

From a crude approximation based on a binary collision, following several authors and looking for the most simple consistent expression, we arrive to the following modelling:

$$I_a = Rab(u_b - u_a) = -R\phi_a$$

where  $R$  is a resistance coefficient, a priori quite independent of the concentration, asymptotically independent of the concentration gradient for small gradients but not necessarily for large ones.

## Refinement

For separated fluids, the concentration gradient becomes infinite and we will see that taking  $\delta$  as a characteristic small size, it can be very convenient to perform a successive modelling of the form:

$$R = R_o(1 + |\delta\nabla a|^2)$$

## Diffusion force

- $F_a = -(nkT)\nabla a$ ,  $F_b = -(nkT)\nabla b$  and  $F = 0$
- Diffusive flux  $\phi_a = -D\nabla a$ , proportional to  $F_a$

## Pressure force

- $F_a = -a\nabla P$ ,  $F_b = -b\nabla P$   $F = -\nabla P$
- Baro-diffusive flux  $\phi_a = \gamma(\rho_a - \rho_b)\frac{ab}{\rho}\nabla P$ , not proportional to  $F_a$ .

## Gravity force

- $F_a = a\rho_a g$ ,  $F_b = b\rho_b g$   $F = \rho g$
- No associated phase flux:  $\phi_a = 0$

## Question

Is there any simple systematic relation?

## Natural split of force pairs

Any phase force can be split in two parts:

- A first part participating to the flow transport as a whole
- A residual part related to the penetration in/separation of the other

To have the first parts "accelerating" the same their respective phase they must be proportional to their mass fraction, according to Newton's law.

## Mathematical formulation

- $F_a = \alpha F + F_0$
- $F_b = \beta F - F_0$
- $\alpha + \beta = 1$
- $\alpha F u_a + \beta F u_b = F u$



## Solution of the Mathematical formulation

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

## Application to the diffusion force

- $F_0 = -(nkT)\nabla a$  for  $\phi_a = -D\nabla a$

## Application to the pressure force

- $F_0 = (\rho_a - \rho_b) \frac{ab}{\rho} \nabla P$  for  $\phi_a = \gamma(\rho_a - \rho_b) \frac{ab}{\rho} \nabla P$

## Application to the gravity force

- $F_0 = 0$  for  $\phi_a = 0$

# "Almost" final modelling assumption

## Statement

The sum of the residual forces  $F_0$  of phase A is in dynamical equilibrium with phase B exchange term.

## Mathematical formulation

$$\Sigma F_0 = I_b$$

## Corrective flux

Direct application of the exchange term modelling gives the volume fraction flux:

$$\phi_a = \frac{1}{R} [(\rho_a - \rho_b) \frac{ab}{\rho} \nabla P + F_0]$$

where now  $F_0$  stands for all the terms proportional to the gradient of concentration. For two perfect gases, we have:  $F_0 = -(nkT)\nabla a$ .

## Statement

- Given a pair of phase potential energies, the force in the momentum equations and the associated corrective flux are uniquely defined.
- Conversely, a force in the global momentum equation together with the associated corrective phase flux uniquely defines both the force in the phase momentum equations and the related potential energies.

## Remark

- This is very convenient because we can freely test any potential
- The Cahn-Hilliard classical formulation is not retrieved, a volume fraction dependent mobility coefficient appears. This is a pity because the Cahn-Hilliard framework has been the main source of inspiration in this work.

## General consideration

While baro-diffusion is a term used for micro-scale, the effect it describes is very general and can be very large scale. Rain and bubbly flows are driven by the mean pressure gradient. Surface tension, by limiting the minimum size of the structure, strengthen the baro-diffusion seen at a larger scale: larger droplets of bubbles have faster drift velocity. Surface tension, however only works at small scale, millimetre range.

There is a formal analogy between the baro-diffusion/surface tension pair and the turbulent dissipation/molecular dissipation. In the later, while the turbulent dissipation makes apparently all the job, only the molecular dissipation effectively lower the kinetic energy. In the former, the separation process is apparently performed by the baro-diffusion, but only the surface tension really separates the phases.

## General consideration

- In the large scale governing equations, the molecular viscosity can be neglected in the bulk flow. By analogy, as in our cases of interest the base cell size is larger than the surface tension range, we can neglect the surface tension effect and concentrate our efforts to the baro-diffusion flux.
- To have a complete phase separation, classical diffusion must be completely cancelled by surface tension anti-diffusion. So, if we neglect surface tension, we also must cancel molecular diffusion.
- In a turbulent framework, turbulent diffusion makes sense. However, its functional form must be changed to avoid unbounded propagation speed and allow stable finite size interface.

# Phase transport equation

## Formula

- First we recognize that  $R = M^{-1}$  where  $M$  is proportional to the classical mobility
- Using the apparent velocity  $v$ , equations symmetrical in  $(a, b)$ :
  - $\partial_t a + \nabla \cdot av - \nabla \cdot Mab(\rho_b - \rho_a) \frac{\nabla P}{\rho} = 0$
  - $\partial_t b + \nabla \cdot bv - \nabla \cdot Mab(\rho_a - \rho_b) \frac{\nabla P}{\rho} = 0$
- Using the mass weighted velocity  $u$ , symmetry is in  $(a\rho_a, b\rho_b)$  but is broken in  $(a, b)$ 
  - $\partial_t a + \nabla \cdot au - \nabla \cdot aM(\rho_b - \rho_a) \frac{b\rho_b}{\rho} \frac{\nabla P}{\rho} = 0$
  - $\partial_t b + \nabla \cdot bu - \nabla \cdot bM(\rho_a - \rho_b) \frac{a\rho_a}{\rho} \frac{\nabla P}{\rho} = 0$

## Remark

- The correction velocity is symmetrical referred to  $v$  and almost entirely concentrated on the light phase when referred to  $u$
- The correction velocity goes to zero with saturation.

# Suggestion for Starccm+ VOF implementation

## Incorporate barodiffusion

- Use phase transport equation with the mass weighted velocity.
- Allow user-defined mobility coefficient  $M$

## Take into account the velocity divergence

- The projection of the velocity  $u$  must be such that:

$$\nabla \cdot u = \nabla \cdot M(\rho_b - \rho_a)^2 \frac{ab}{\rho} \frac{\nabla P}{\rho}$$

## Remark

- The baro-diffusion term should allow to consistently consider phase change (evaporation or condensation) without large interface smearing in case of evaporation. The velocity divergence becomes:

$$\nabla \cdot u = \left(1 - \frac{\rho_b}{\rho_a}\right) \dot{S}_b + \nabla \cdot M(\rho_b - \rho_a)^2 \frac{ab}{\rho} \frac{\nabla P}{\rho}$$

where  $\dot{S}_b$  is the volume rate of created gas.

# Impossible for end-user to force the variant in Starccm+ VOF

## Problem in mass conservation

The baro-diffusion term should be of null integral over a volume enclosing the free-surface, the flux being null at the boundary. Setting the baro-diffusion term as a source term in Starccm+, we have encountered a relative error about 12%:

$$\frac{|\int_{\Omega} \nabla \cdot \frac{ab\nabla P}{\rho^2}|}{\int_{\Omega} |\nabla \cdot \frac{ab\nabla P}{\rho^2}|} \sim 12\%$$

and thus the total phase volume is not conserved (the effect is quite strong). This come from the fact that the numerical discretization of a source which is the divergence of a flux do not comply with the Stokes theorem (while classical diffusion flux should do).

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## Millimetre range application

When the discretization reaches the millimetre range. Surface tension may become relevant. The Cahn-Hilliard framework being reserved to scales at least one order less. The energy leading to the Landau surface tension force is:

- $E_a = \int_{\Omega} \sigma b |\nabla a|$ ,  $E_b = \int_{\Omega} \sigma a |\nabla b|$ ,  $E = \int_{\Omega} \sigma |\nabla a|$ .
- $F = -\sigma \nabla \cdot n \nabla a$ ,
- $F_0 = \sigma a b \nabla \nabla \cdot n + \frac{ab}{\rho} (\rho_b - \rho_a) F$
- The first RHS term of  $F_0$  serves to regularize the curvature. It is degenerated when a local extrema of  $a$  is not zero or one. At the foreseen level of description, it may be wiser to discard the term.
- The second RHS term of  $F_0$  is quite similar to the baro-diffusion term and seems to indicate that no baro-diffusion should occur if the pressure gradient is caused by a curvature effect. This term seems to make sense.

## Millimetre range application

We can see that this surface tension energy is quite neutral for what concern diffusion effect but is still marginally diffusive in presence of curvature. In the Cahn-Hilliard framework, the constitutive energy (only globally defined) is:

- $E = \frac{1}{2} \int_{\Omega} [\alpha |\nabla a|^2 + \beta a^2 b^2]$ .
- We could not find any elegant splitting giving both  $F$  and  $F_0$  pleasant.
- The first RHS term of  $E$  has a clear diffusing effect while the second one has a clear contracting effect.
- Moreover, the minimum of the second part is clearly reached for perfectly separated fluids
- looking for the analogy of form, it is tempting to consider an energy in which the "2" are transformed in "1".

## Millimetre range application

The effect is to include a contracting energy in the Landau surface tension energy, that is adding the energy:

- $E = \int_{\Omega} \sigma \frac{ab}{\delta}$  where  $\delta$  is a characteristic length over which the related force is relevant against curvature.
- We could find the splitting:  $E_a = \int_{\Omega} \sigma \frac{ab(1+b)}{3\delta}$ ,  $E_b = \int_{\Omega} \sigma \frac{ab(1+a)}{3\delta}$
- for which  $F = 0$ , so no added term in the momentum equation and
- $F_0 = 2\sigma \frac{ab}{\delta} \nabla a$
- To avoid an inconsistent unbounded drift velocity for large gradients, one can take the resistance term  $R$  as:  $R = R_0(1 + |\delta \nabla a|^2)$  so that the drift velocity gently goes to zero while the interface strongly sharpens.

## Remark

The symmetrization of the contracting part of the energy is needed to avoid an increase of pressure across a flat interface. In alternative, one can revert to a higher power term (e.g.  $a^2 b^2$ ).






## Sardinia Autonomous Region

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## Main sources of inspiration

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Greetings

Thank you for your attention

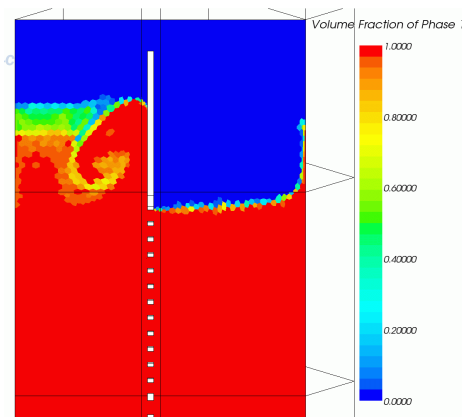


Figure: Nice interface smearing combining oscillatory motion and shear