

Derivation of continuity equation in VOF with mass transfer

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November 25, 2015

VOF is defined as volume averaged equations where the control volume is a cell of the domain. To derive the continuity equations with and without mass transfer, one first needs to define the physical problem, the cell-based average and some theorem to derive averaged (or filtered) equations.

1 Physical problem

We start with the physics, without thinking about numerics. There are two mass balance equations, one in each domain. For the domain, V_l , occupied by liquid, we have:

$$\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{v}_l) = 0 \text{ in } V_l, \quad (1)$$

and for the domain, V_g , that contains gas:

$$\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{v}_g) = 0 \text{ in } V_g. \quad (2)$$

These equations are completed with boundary conditions at Γ_{lg} , the liquid/gas interface:

$$\mathbf{n}_{lg} \cdot \rho_l (\mathbf{v}_l - \mathbf{w}) = \mathbf{n}_{lg} \cdot \rho_g (\mathbf{v}_g - \mathbf{w}) \text{ at } \Gamma_{lg} \quad (3)$$

where \mathbf{w} is the velocity of the interface.

Here we can define the phase indicator χ_l as:

$$\chi_l = \begin{cases} 1 & \text{in } V_l \\ 0 & \text{in } V_g \end{cases}. \quad (4)$$

Numerically with VOF, we deal with a grid-based physics. Which means that a cell of the domain can contain both gas and liquid. Because of that, χ_l is not relevant, and one need to define cell-averaged properties.

2 Average and averaging theorems

We introduce a computational grid and we define two different averages that also can be seen as average operators. The superficial average (averaged over the cell volume V):

$$\langle \phi_l \rangle = \frac{1}{V} \int_{V_l} \phi_l dV,$$

and the intrinsic phase average (averaged over the volume of liquid V_l contained in the cell):

$$\langle \phi_l \rangle^l = \frac{1}{V_l} \int_{V_l} \phi_l dV.$$

Applying the average operator $\langle \cdot \rangle$ to the phase indicator χ_l gives

$$\langle \chi_l \rangle = \varepsilon_l,$$

which is the color function used in VOF (when $\varepsilon_l = 1$ the cell is full of liquid, $\varepsilon_l = 0$ the cell is full of gas, and intermediate values denote the interface). Note that both averages are related by: $\langle \phi_l \rangle = \varepsilon_l \langle \phi_l \rangle^l$.

To derive the governing equations of the average properties, the following theorem are used for the integral-derivative inversion:

$$\left\langle \frac{\partial \phi_l}{\partial t} \right\rangle = \frac{\partial \langle \phi_l \rangle}{\partial t} - \frac{1}{V} \int_{\Gamma_{lg}} \mathbf{n}_{lg} \cdot \mathbf{w} \phi_l d\Gamma,$$

and

$$\langle \nabla \cdot \mathbf{b}_l \rangle = \nabla \cdot \langle \mathbf{b}_l \rangle + \frac{1}{V} \int_{\Gamma_{lg}} \mathbf{n}_{lg} \cdot \mathbf{b}_l d\Gamma.$$

3 Derivation

To derive the governing equations for the grid-based domain, we apply the averaging theorem to the physical problem described in the first Section. It gives,

$$\frac{\partial \langle \rho_l \rangle}{\partial t} + \nabla \cdot (\langle \rho_l \mathbf{v}_l \rangle) + \frac{1}{V} \int_{\Gamma_{lg}} \mathbf{n}_{lg} \cdot \rho_l (\mathbf{v}_l - \mathbf{w}) d\Gamma = 0, \quad (5)$$

We can define the mass transfer rate from the liquid to gas phase as:

$$\dot{m} = \frac{1}{V} \int_{\Gamma_{lg}} \mathbf{n}_{lg} \cdot \rho_l (\mathbf{v}_l - \mathbf{w}) d\Gamma, \quad (6)$$

which give:

$$\frac{\partial \varepsilon_l \langle \rho_l \rangle^l}{\partial t} + \nabla \cdot (\varepsilon_l \langle \rho_l \mathbf{v}_l \rangle^l) = -\dot{m}. \quad (7)$$

Similarly, we can derive the mass conervation for the gas phase:

$$\frac{\partial \varepsilon_g \langle \rho_g \rangle^g}{\partial t} + \nabla \cdot (\varepsilon_g \langle \rho_g \mathbf{v}_g \rangle^g) = \dot{m} \quad (8)$$

At that point of the development, we introduce the assumption of incompressibility for both phases: ρ_i is constant within the control volume, i.e. $\langle \rho_i \rangle^i = \rho_i$ and that $\langle \rho_i \mathbf{v}_i \rangle^i = \rho_i \langle \mathbf{v}_i \rangle^i$. Hence, these two equations are recast into:

$$\frac{\partial \varepsilon_l}{\partial t} + \nabla \cdot (\varepsilon_l \langle \mathbf{v}_l \rangle^l) = -\frac{\dot{m}}{\rho_l} \quad (9)$$

$$\frac{\partial \varepsilon_g}{\partial t} + \nabla \cdot (\varepsilon_g \langle \mathbf{v}_g \rangle^g) = \frac{\dot{m}}{\rho_g} \quad (10)$$

In the VOF method, there is no equation for $\langle \mathbf{v}_l \rangle^l$ and $\langle \mathbf{v}_g \rangle^g$ but there are equations for the velocity field $\langle \mathbf{v} \rangle = \varepsilon_l \langle \mathbf{v}_l \rangle^l + \varepsilon_g \langle \mathbf{v}_g \rangle^g$. Since $\varepsilon_g + \varepsilon_l = 1$, we can also write $\langle \mathbf{v} \rangle = \varepsilon_l \langle \mathbf{v}_l \rangle^l + (1 - \varepsilon_l) \langle \mathbf{v}_g \rangle^g$ which is the classic definition of the velocity in VOF method. The addition of these two equations give the global mass balance equation:

$$\nabla \cdot \langle \mathbf{v} \rangle = \dot{m} \left(\frac{1}{\rho_g} - \frac{1}{\rho_l} \right). \quad (11)$$

The right hand side of this equation denotes the mass transfer between the two phases. It is non-zero only at the gas/liquid interface ($0 < \varepsilon_l < 1$).

The other equation that needs to be derived is the equation for the color function ε_l . Indeed, Eq (9) cannot be used directly because it depends on $\langle \mathbf{v}_l \rangle^l$ and VOF only solves $\langle \mathbf{v} \rangle$. With simple algebra, this equation can be recast into:

$$\frac{\partial \varepsilon_l}{\partial t} + \nabla \cdot (\varepsilon_l (\varepsilon_g + \varepsilon_l) \langle \mathbf{v}_l \rangle^l) = -\frac{\dot{m}}{\rho_l}, \quad (12)$$

$$\frac{\partial \varepsilon_l}{\partial t} + \nabla \cdot (\varepsilon_l \varepsilon_l \langle \mathbf{v}_l \rangle^l) + \nabla \cdot (\varepsilon_l \varepsilon_g \langle \mathbf{v}_l \rangle^l) = -\frac{\dot{m}}{\rho_l}, \quad (13)$$

$$\frac{\partial \varepsilon_l}{\partial t} + \nabla \cdot (\varepsilon_l \varepsilon_l \langle \mathbf{v}_l \rangle^l + \varepsilon_l \varepsilon_g \langle \mathbf{v}_g \rangle^g) + \nabla \cdot (\varepsilon_l \varepsilon_g \langle \mathbf{v}_l \rangle^l - \varepsilon_l \varepsilon_g \langle \mathbf{v}_g \rangle^g) = -\frac{\dot{m}}{\rho_l}, \quad (14)$$

that finally gives,

$$\frac{\partial \varepsilon_l}{\partial t} + \nabla \cdot (\varepsilon_l \langle \mathbf{v} \rangle) + \nabla \cdot (\varepsilon_l (1 - \varepsilon_l) \langle \mathbf{v}_r \rangle) = -\frac{\dot{m}}{\rho_l}. \quad (15)$$

This is the equation for the indicatrice function solved in OpenFOAM. In this equation, the last term of the left hand side corresponds to the compressibility

of the interface. This term is non-zero only at the gas/liquid interface. The relative velocity, $\langle \mathbf{v}_r \rangle = \langle \mathbf{v}_l \rangle - \langle \mathbf{v}_g \rangle$ is approximated based on the maximum value of $\langle \mathbf{v} \rangle$ at the fluids interface.

4 Momentum equation

Same strategy can be adopted to derive the momentum equation for $\langle \mathbf{v} \rangle$. That way, the CSF force appears naturally.