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Formulation of fully implicit method for simulation of flows with interfaces using primitive variables

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ABSTRACT

This paper is concerned with simulation of flows with *interface* between two incompressible and immiscible fluids on a fixed grid using what is called the *single fluid formalism*. This formalism views flow of two fluids as that of a single fluid whose density and viscosity change abruptly at the interface. The location of the interface is *apriori* not known but is to be discovered as part of the solution. Problems of this type are typically solved using an equation for (a) Volume Fraction or, for (b) Level Set function. In the present paper, the governing Navier–Stokes equations in primitive variables are solved on collocated grids using SIMPLE algorithm with a specially derived *smoothing pressure correction* that satisfies *volume conservation*. A *superficial density* is defined and determined from *mass conservation* equation. It is shown that this equation can be cast in the form of a well-known *volume fraction* equation. The interface location is determined without interface reconstruction. The convective terms are represented by a TVD scheme to predict less-smeared interface. The surface tension force is evaluated by two methods via *geometric* and *fluid dynamic* evaluation of the interface curvature.

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1. Introduction

Numerical prediction of unsteady flow of two incompressible and immiscible fluids has been a subject of intense research since the publications of Harlow and Welsh [1] who used the Marker-and-Cell (MAC) method employing staggered arrangement of vector and scalar variables. In order to capture the interface, one of the fluids is identified by marker particles. The momentum equations are solved by explicit method. Hirt and Nicolls [2] introduced the *Volume of Fluid* (VOF) method in which an *Advection* equation

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + u_j \frac{\partial F}{\partial x_j} = 0 \tag{1}$$

is *postulated* for predicting the distribution of volume fraction F of the *heavier fluid* in space and time. Some geometric properties of the interface are derived from the local F distribution so as to facilitate evaluation of convective fluxes according to the *donor–acceptor* principle. In more recent times several new interface reconstruction techniques have been used [8–11].

The publication of Jun and Spalding [3] is of a similar kind but employed the SIMPLEST algorithm in which, at every time step, the momentum and pressure-correction equations are solved on a staggered grid implicitly whereas the interface is tracked by solving (using the fully-explicit van-Leer scheme [4]) an equation for a *conserved scalar* (CS) Φ,

$$\frac{\partial \Phi}{\partial t} + \frac{\partial \Phi u_j}{\partial x_j} = 0 \tag{2}$$

This equation is same as the advection Eq. (1) for the volume fraction F when continuity equation ($\partial u_j/\partial x_j = 0$) is invoked for incompressible fluids. More recently, Andrillon and Alessandrini [5] have employed the CICSAM scheme (a variant of a TVD scheme obeying the NVD principle [7]) due to Ubbink and Issa [6] for the solution of the conserved scalar equation on unstructured meshes using collocated variables. The momentum and the conserved scalar equation are solved by semi-implicit Crank–Nicholson method. Another variant in this type of interface capturing methods is the Flux Corrected Transport (FCT)-VOF method due to Rudman [19].

Another class of interface capturing methods employ the *Level-Set* (LS) method [12] in which the advection equation is written for the *signed interface distance function* Ψ whose distribution in an unsteady problem is re-initialised at each time-step by requiring that $|\nabla \Psi| = 1$ [13]. The form of the Ψ-equation is same as the Φ-equation mentioned above. In order to conserve mass, particularly at larger times of interface movement, Zhang et al. [15], among others (see, for example, [16,17,14,20]), have introduced modifications to this method. Some of these methods have shown

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Nomenclature

AE, AW, AN, AS, AP	coefficients in discretised equations
F	volume fraction
Fr	Froude number
F_{st}	surface tension force
p	pressure
q	invariant component of normal stress
R	residual
Re	Reynolds number
S	source term
t	time
u_i	velocity in $x_i, i = 1, 2, 3$ direction
V	volume
$\vec{V}$	total velocity vector
We	Weber number

Greek symbols

α	under-relaxation factor
Δ	incremental value
μ	dynamic viscosity
ρ	density
Φ	conserved scalar or General Variable
Ψ	distance function
λ_1	multiplier of $p - \bar{p}$
σ	normal stress or surface tension coefficient

Suffixes

P, N, S, E, W	refers to grid nodes
m	refers to mass conservation
n	normal to the interface
sm	refers to smoothing
x_i	refers to $x_i, i = 1, 2, 3$ directions

Superscripts

l	iteration counter
o	old time
u_i	refers to momentum equations
$-$	multidimensional average
$\prime$	correction

ability to predict liquid break-ups and fine fluid atomisations. The momentum and the distance-function equation are often discretised by very high order ENO/WENO schemes. This completely mathematical method is considered most accurate for predicting interfacial flows [21] and has found adherents in combustion (flame-tracking) and phase-change (melting and solidification) applications as well.

A third approach relies on *geometric reconstruction* of the interface on the basis of predicted distributions of the volume fraction F. In papers by Rudman [19] and Gerlach et al. [23], several methods of this type have been compared on 2-dimensional problems. Such methods (see also [24]), however, prove to be very cumbersome when 3-dimensional problems are considered on structured or unstructured meshes.

In this paper, we present a formulation of multi-dimensional problems with and without surface tension force using an approach which relies on the faith that the Navier–Stokes equations in *primitive variables* contain all the necessary information for prediction of the interface locations and neither geometric interface-reconstruction nor mathematical level-set formulation are invoked. The present formulation is equally applicable to problems on structured or unstructured meshes.

Finally, it is important to recognise that all methods require extremely fine meshes to resolve fine flow structures that occur when fluid splits (atomisation) or tiny bubble entrapments in liquid occur. Adaptive grid generation techniques overcome this need for very fine grids by embedding additional cells in regions where grid-fineness is required. But, in an unsteady calculation where the interface locations are continuously changing, this means that adaptive procedures must be programmed for both adding as well as for deleting computational cells. Such methods achieve economy [25,26]. Thus, the problem of accurately predicting interfacial flows is computationally very demanding requiring continuous improvements both in physics of modeling as well as in solvers used for discretised equations. The latter are not reviewed here. Our approach in this paper is to remain as close to single fluid flow algorithms as possible with easily adaptable changes to existing generalised fixed-grid computer codes devised for single fluid flows.

2. Present formulation

2.1. Governing equations

Within the *single fluid formalism*, the unsteady flow of two incompressible immiscible fluids is governed by the following equations.

$$\frac{\partial u_j}{\partial x_j} = \nabla \cdot \vec{V} = 0 \tag{3}$$

$$\frac{\partial \rho_m u_i}{\partial t} + \frac{\partial \rho_m u_j u_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\mu_m \frac{\partial u_i}{\partial x_j}\right] - \frac{\partial p}{\partial x_i} + \rho_m g_i + F_{st,i} + \frac{\partial}{\partial x_j}\left[\mu_m \frac{\partial u_j}{\partial x_i}\right] \tag{4}$$

Eq. (3) represents *volume conservation* whereas Eq. (4) represents momentum equations in *conservative form*. $F_{st,i}$ is the surface tension force and g_i is the gravitational acceleration. Most importantly, ρ_m is a *superficial density* associated with the interface which represents a plane of *discontinuity* between heavier fluid a and lighter fluid b. ρ_m equals ρ_b or ρ_a within each fluid.

Eqs. 3 and 4 can be derived from conventional control-volume analysis. They define the fluid motion completely when procedures for evaluating superficial properties ρ_m and μ_m and the surface tension force $F_{st,i}$ are formulated.

2.2. Evaluation of ρ_m and μ_m

Consider a 2-dimensional Cartesian control-volume (CV) shown in Fig. 1. The figure shows a CV in which the interface resides (solid line) at time t. Then the total mass of CV is $M = m_a + m_b$ and the total volume is $V = V_a + V_b$. Hence, the superficial density for this CV will evaluate to

$$\rho_m = \frac{m_a + m_b}{V} = \frac{\rho_a V_a + \rho_b V_b}{V} = \rho_a \frac{V_a}{V} + \rho_b \frac{V_b}{V} \tag{5}$$

If we now define the volume-fraction of the *heavier fluid* as

$$F \equiv \frac{V_a}{V} \tag{6}$$

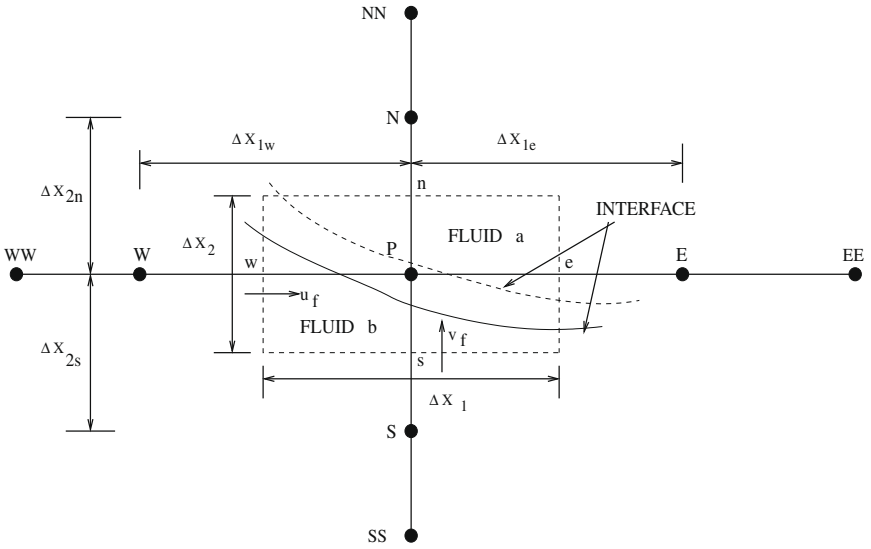

Fig. 1. A control volume with an interface.

then the volume fraction of the lighter fluid will be $V_b/V = 1 - F$. As such, the superficial density will read as

$$\rho_m = \rho_a F + \rho_b(1 - F) \tag{7}$$

or, the volume fraction F can also be defined as

$$F \equiv \frac{V_a}{V} = \frac{\rho_m - \rho_b}{\rho_a - \rho_b} \tag{8}$$

This equation shows that $F = 1$ (with $\rho_m = \rho_a$) in the heavier fluid and $F = 0$ (with $\rho_m = \rho_b$) in the lighter fluid. The exact value of F *at the interface*, however, remains unknown being multi-valued. That is, at the interface, $0 < F < 1$. By resorting to pragmatism, however, $F = 0.5$ can be taken as the exact location of the interface as is the usual practice. As such, in a discretised space, the predicted F distribution will appear *smeared* in the neighbourhood of $F = 0.5$.

Further, with respect to Fig. 1, it will be recognised that a new time $(t + \Delta t)$, the interface will move to a new position (dotted line). At any new time, while V_a and V_b will have changed, $V = V_a + V_b$ will remain constant; thus justifying Eq. (3). But, the total mass $M = m_a + m_b$ in the CV will have changed. As such, the superficial density ρ_m and hence, F will have changed. It is this change that via control-volume analysis is reflected in Eq. (9).

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_j}{\partial x_j} = 0 \tag{9}$$

This equation determines superficial density distribution with time from which volume fraction F can be determined using Eq. (8). The justification for this equation has also been given in the book by Durbin and Medic [32]; albeit without derivation. Further, superficial viscosity, being a transport property, may be evaluated by volume fraction weighting as

$$\mu_m = \mu_a F + \mu_b(1 - F) \tag{10}$$

2.2.1. The VOF and Conserved-Scalar Equation

In the derivation above, volume fraction F is derived from density rather than the other way round as is the practice in VOF, CS and LS methods. It is therefore of interest to demonstrate how Eq. (9) represents VOF and conserved-scalar equations. Thus, using Eqs. 7 and 3, Eq. (9) can also be re-written as

$$\frac{\partial F}{\partial t} + \frac{\partial u_j F}{\partial x_j} = -\frac{\rho_b}{\rho_a - \rho_b}\frac{\partial u_i}{\partial x_i}^{=0} = 0 \tag{11}$$

This equation which is same as conserved scalar Eq. (2), essentially represents mass- and volume-conservation simultaneously. Many authors solve this equation in lieu of Eq. (9) to recover density and viscosity. Thus, in the conserved scalar approach, Eq. (11) is solved in addition to the volume-conservation Eq. (3) which is deployed to recover pressure. On the other hand, by using Eq. (3) again, Eq. (11) can be further reduced to VOF- Eq. (1). In the VOF method, Eq. (1) is *simply postulated* and not derived. In this method, it is believed that the interface location can be tracked by evaluating the volume-fraction F of the heavier fluid. Finally, note that like in Eq. (9), there are no diffusion terms in Eq. (11) and the source term is zero.[1]

Thus, within the Single Fluid Formalism, Eqs. 3, 4 and 9 (or 11) provide the complete set of equations to be solved. The equation set is unique because it draws on continuity Eq. (3) invoked in incompressible flow as well as on mass-conservation Eq. (9) that is invoked in compressible fluid flows. This is necessitated because when both fluids are incompressible, there is no equation-of-state available to connect density to pressure. In this respect, it is worth noting that in one approach called the *ghost-fluid formulation* [22], an equation-of-state for water is invoked along with the perfect gas-law for air. In the present formulation, Eq. (3) is used for recovery of pressure whereas Eq. (9) is used for recovering ρ_m (or F) distributions without using any equation of state. This approach has affinity to that employed by Jun and Spalding [3].

[1] In the LS method, the interface locations are assigned a constant value (usually zero). The equation governing evolution of this level set is then simply $D\Psi/Dt = 0$. Using Eq. (3), however, a conservative equation having the form of Eq. (11) can again be derived but variations of Ψ are restricted to $-d \leqslant \Psi \leqslant d$ where d is of the order of mesh size used in the computations. This, unlike F, makes Ψ a signed distance function that needs to be re-initialised at every time step. Thus, although similar in form, the F and Ψ equations have different meanings. Interface smearing is present in VOF as well as LS methods but the smearing width is restricted in the LS method.

2.3. Method of solution

Unlike all publications accessible to us for solving the class of problems considered in this paper, we follow the ideas embodied in SIMPLE algorithm by Patankar and Spalding [27]. In this algorithm, the unsteady flows are also to be calculated by solving the momentum, pressure correction and any scalar equations in *fully implicit* manner at every time step on a *staggered grid*. Here, however, we implement the SIMPLE algorithm on *collocated grids* while retaining fully-implicit treatment. For this purpose, Eqs. 3, 4 and 9 (or, Eq. (11)) are represented by the following equation for a general variable $\Phi = u_1, u_2$ and ρ_m or F[2]

$$\frac{\partial(\rho_m \Phi)}{\partial t} + \frac{\partial(\rho_m u_j \Phi)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\mu_m \frac{\partial \Phi}{\partial x_j}\right] + S_\Phi \tag{12}$$

With reference to Fig. 1, for a two-dimensional flow, the Finite-Volume discretisation of Eq. (12) yields an implicit equation (see [28]) for any node P

$$(BP + AP)\Phi_P^{l+1} = AW\Phi_W^{l+1} + AE\Phi_E^{l+1} + AS\Phi_S^{l+1} + AN\Phi_N^{l+1} + BP\Phi_P^{o} + S_\Phi^{l} + S_{tvd}^{l} \tag{13}$$

where superscript l represents the iteration number, superscript o represents *old time* values and

$$AP = AE + AW + AN + AS \tag{14}$$

$$AE = 0.5(|C_e| - C_e) + d_e \quad AW = 0.5(|C_w| + C_w) + d_w \text{ etc} \tag{15}$$

$$C_e = (\rho_m u \Delta x_2)_e \quad d_e = \mu_e \frac{\Delta x_2}{\Delta x_{1e}} \tag{16}$$

$$C_w = (\rho_m u \Delta x_2)_w \quad d_w = \mu_w \frac{\Delta x_2}{\Delta x_{1w}} \tag{17}$$

$$BP = \frac{\rho_{m,P}^{o} \Delta V}{\Delta t} \tag{18}$$

$$S_\Phi = \text{Source Term} \times \Delta V \tag{19}$$

$$S_{tvd} = \text{TVD Source Term} \times \Delta V \tag{20}$$

The representation of the time derivative is first order accurate. Variation of all variables between adjacent nodes is assumed linear. As such, the discretisation of the diffusive fluxes is second order accurate. Following Date [28,30], the total convective flux is represented as a sum of the flux according to first order UDS (shown in Eq. (15)) and a correction TVD flux that imparts high order accuracy and reduces the amount of numerical smearing associated with 1st order UDS. Thus, the S_{tvd}^{l} term that lags by one iteration, represents the corrective convection fluxes that are given by

$$\begin{aligned} S_{tvd} = {} & \frac{1}{2}(Ce + |Ce|) f_{ce}^{+}(\Phi_W - \Phi_E) + \frac{1}{2}(Ce - |Ce|) f_{ce}^{-}(\Phi_{EE} - \Phi_P) \\ & + \frac{1}{2}(C_w + |C_w|) f_{cw}^{+}(\Phi_P - \Phi_{WW}) + \frac{1}{2}(C_w - |C_w|) f_{cw}^{-}(\Phi_W - \Phi_E) \\ & + \frac{1}{2}(Cn + |Cn|) f_{cn}^{+}(\Phi_S - \Phi_N) + \frac{1}{2}(Cn - |Cn|) f_{cn}^{-}(\Phi_{NN} - \Phi_P) \\ & + \frac{1}{2}(Cs + |Cs|) f_{cs}^{+}(\Phi_P - \Phi_{SS}) + \frac{1}{2}(Cs - |Cs|) f_{cs}^{-}(\Phi_S - \Phi_N) \end{aligned} \tag{21}$$

where the fc's are the *shape-sensing* functions of the form

$$f_c(\xi) = f_c\left(\frac{\Phi_U - \Phi_{UU}}{\Phi_D - \Phi_{UU}}\right) \tag{22}$$

Here, D connotes downstream, U connotes upstream and UU is upstream of U. Thus, at cell face e, for example, f_{ce}^{+} is a function of $(\Phi_P - \Phi_W)/(\Phi_E - \Phi_W)$ when Ce is positive, and, likewise, f_{ce}^{-}, is a function of $(\Phi_E - \Phi_{EE})/(\Phi_P - \Phi_{EE})$ when Ce is negative. In the scheme due to Lin and Lin [37] adopted here, the function $f_c(\xi)$ is as given in Table 1.

Table 1
Function $f_c(\xi)$ [37].

Range of ξ	f_c
$\xi \ni [0, 1]$	0
$\xi \in [0, 0.3]$	ξ
$\xi \in [0.3, 5/6]$	$3/8 - \xi/4$
$\xi \in [5/6, 1]$	$1 - \xi$

This TVD scheme obeys the NVD principle [7]. Date [28,30] has used this scheme for a problem of compressible shock prediction. It's application to flows with interfaces is new. In different TVD schemes (see [38–41,21], for example), the function $f_c(\xi)$ are different.

2.4. Calculation procedure

The overall fully-implicit calculation procedure is as follows:

1. Specify problem dependent initial conditions of F, u_1 and u_2. Hence evaluate ρ_m and μ_m.
2. Choose a time step Δt.
3. Guess pressure p^l and evaluate problem dependent source terms such as $\rho_m g_i$ and $F_{st,i}$ (see Section 2.6). Carry out one iteration of momentum equation to yield u_i^l distributions.
4. Set-up pressure correction equation on the basis of *volume conservation* Eq. (3). Thus, following Date [28,29], solve *for total pressure correction* p'

$$\frac{\partial}{\partial x_j}\left[\frac{\alpha \Delta V}{(AP + BP)^{u_j}} \frac{\partial p'}{\partial x_j}\right] = \frac{\partial \bar{u}_j^l}{\partial x_j} \tag{23}$$

   where $\bar{u}_j^l$ are average of nodal velocities at the control-volume faces and α is the under-relaxation factor used in momentum equations. In general, $\bar{u}_j^l$ do not satisfy momentum equations over the control volumes surrounding the cell-faces. This creates need for introducing a *smoothing pressure correction* p'_{sm} [28,29].
5. Perform 10 iterations on Eq. (23) to yield p' distribution. The mass/volume-conserving pressure correction is now recovered as

$$p'_{m,P} = p'_P - p'_{sm,P} \tag{24}$$

   Further derivation of the smoothing pressure correction p'_{sm} from *fluid-dynamic* considerations is described in Section 2.5.
6. Correct pressure and velocities as

$$p_P^{l+1} = p_P^l + 0.1 \times p'_{m,P}$$
$$u_{j,P}^{l+1} = u_{j,P}^l - \frac{\Delta V}{(AP + BP)^{u_j}} \left.\frac{\partial p'_m}{\partial x_j}\right|_P \tag{25}$$

7. Solve F- Eq. (11) or ρ_m Eq. (9). Hence, evaluate fluid property μ_m.
8. Check for convergence by evaluating residual defined as

$$R_\Phi \equiv \frac{1}{(J\Phi)_{in}}\left[\sum_{allnodes} \{\text{Imbalance in Eq.(13)}\}^2\right]^{0.5} < \text{CC} \tag{26}$$

where $(J\Phi)_{in}$ is the inlet-flux of Φ and CC is a small number.[3] If convergence is not satisfied, return to step 3 to carry out further iterations.

[2] $\Phi = 1$ when Eq. (9) is solved. If Eq. (11) is solved, ρ_m is set to 1. The right hand side is zero in both equations.

[3] CC is set to 10^{-5} in all problems. However, in problems in which surface tension is included, R_Φ is further divided by number of control volumes in the domain. This is also found necessary by Takahira [16] to satisfy the convergence criterion CC = 10^{-5}. Also, note that if there is no inlet flux present then $(J\Phi)_{in}$ is set to 1.

9. Set $\Phi^o = \Phi$ and return to step 2 to execute the next time step.

Thus, except for step 5 where p'_m is recovered from p', the present algorithm is the same as that used in the original SIMPLE algorithm on staggered grid. All equations are solved by ADI method using under-relaxation factor $\alpha = 1$ in momentum and F equations and $\alpha \leqslant 1$ in p' equation as per the need.

2.5. Evaluation of p'_{sm}

Schlichting [33] and Warsi [34] have defined a quantity $\bar{p}$ as follows

$$\bar{p} = -\frac{1}{3}(\sigma_{x_1} + \sigma_{x_2} + \sigma_{x_3}) \tag{27}$$

where σ_{xi} are normal stresses.[4] Now, an often overlooked requirement of the Stokes's law relating the stress to the rate-of-strain is that, in a continuum, $\bar{p}$ must equal the point value of pressure p. That is

$$\bar{p} = p \tag{29}$$

This requirement holds even when fluid properties vary in an arbitrary manner. Of course, the requirement assumes that there are *no relaxation processes at work* at the molecular level. In single fluid formalism the above conditions are indeed satisfied. As such, substituting for σ,

$$\bar{p} = p - q - \frac{2}{3}\mu\nabla\cdot\vec{V} \tag{30}$$

where q is a newly defined quantity.[5] It is defined to satisfy the requirement of Stokes's law. That is,

$$p'_{sm} = q \tag{31}$$

q = 0 in a continuum. However, in a discretised space, q must be *appropriately chosen* to render $\bar{p} = p$ [28]. We consider different cases of fluid flow to derive q.

1. *Case 1:* ($\vec{V} = 0$) In this *hydrostatic case*,

$$\bar{p} = p - q \tag{32}$$

But in this case, p can only vary linearly with x_1, x_2, x_3 and, therefore, the point value of p exactly equals its space averaged value $\bar{p}$ in both continuum as well as discretised space and hence $p'_{sm} = q = 0$ exactly.

2. *Case 2:* ($\mu = 0$ or $\nabla\cdot\vec{V} = 0$) Clearly when $\mu = 0$ (inviscid flow) or $\nabla\cdot\vec{V} = 0$ (constant density incompressible flow) Eq. (32) again holds. But, in this case, since fluid motion is considered, p can vary arbitrarily with x_1, x_2, x_3 and, therefore, p may not equal $\bar{p}$ in a discrete space. For this case, Date [28] has shown that without violating the continuum requirement, we may set

$$p'_{sm} = q = \lambda_1(p - \bar{p}) \tag{33}$$

where λ_1 is an arbitrary constant. In most textbooks, where continuum is assumed, λ_1 is trivially set to zero. This case applies to regions where F = 0 or 1 (single fluid control volumes) and is of importance to eliminate the problem of zig-zag pressure prediction on collocated grids. Although λ_1 is an arbitrary constant, the analysis of the discretised equations show that $\lambda_1 = 1/2$ [28]. This method of eliminating zig-zag pressure prediction is different from the momentum interpolation method used by Rhie and Chow [35] or Ferziger and Peric [36].

3. *Case 3:* ($\mu \neq 0$ and $\nabla\cdot\vec{V} \neq 0$) This case represents either compressible flow where density is a function of both temperature and pressure or incompressible flow in which density may depend on any scalar quantity such as temperature or void fraction F. This case is of special relevance in regions where $0 < F < 1$ (Control volumes containing the interface) and the superficial density varies with F.

In this case, Stokes's requirement will be satisfied if we set

$$q = \lambda_1(p - \bar{p}) - \frac{2}{3}\mu\nabla\cdot\vec{V} \tag{34}$$

However, note that in a discretised space, in the region $0 < F < 1$, $\nabla\cdot\vec{V} \neq 0$ because density varies in space and time and μ is also finite. But, in a continuum, from Eq. (9) it follows that

$$\nabla\cdot\vec{V} = -\frac{D}{Dt}(\ln\rho_m) = -\left[\frac{\partial}{\partial t}(\ln\rho_m) + u_j\frac{\partial}{\partial x_j}(\ln\rho_m)\right] \tag{35}$$

Therefore, substituting Eq. (35) in Eq. (34), we have

$$p'_{sm} = q = \frac{1}{2}(p - \bar{p}) + \frac{2}{3}\mu\left[\frac{\partial}{\partial t}(\ln\rho_m) + u_j\frac{\partial}{\partial x_j}(\ln\rho_m)\right] \tag{36}$$

The first term on the right hand side represents difference between point value and the local space averaged value of pressure. It ensures that the problem of zig-zig pressure field prediction is eliminated. The second term which is influenced by viscosity, represents the effect of *rate of volume change*. If this term is not nullified (or, accounted for) then the system will experience *dissipation* even when the temperature remains constant. This is, of course, improbable.[6] Here, non-nullification results in loss of volume and, hence, mass. Thus, the second term is of importance for ensuring volume/mass conservation during the entire transient process. The term is identically zero when F = 0 or 1 (over 3 neighbouring CVs in each direction in a discretised space) and Eq. (33) is readily recovered. Thus, since Eq. (36) is applicable to all regions of flow, it is used to evaluate smoothing pressure correction in the present calculations. To the best of our knowledge, this manner of avoiding the problem of *loss of mass* (within discretisation errors) is a new contribution to fluid dynamics of incompressible flows with interfaces.

4. Finally, as shown in Date [28], the space-averaged pressure is evaluated as

$$\bar{p}_P = \frac{1}{3}(\bar{p}_{x_1} + \bar{p}_{x_2} + \bar{p}_{x_3})_P \tag{37}$$

where

$$(\bar{p}_{x_i})_P = \text{solution to } \frac{\partial^2 p}{\partial x_i^2}|_P = 0 \tag{38}$$

This manner of evaluation[7] of $\bar{p}_P$ is directly applicable to computations on both structured and unstructured meshes.

[4] The expression for the normal stress is given by

$$\sigma_{xi} = -p + q + \tau_{ii} \quad \tau_{ii} = 2\mu\frac{\partial u_i}{\partial x_i} \text{ no summation.} \tag{28}$$

[5] The quantity q must be invariant under rotation of the coordinate system or interchange of axes [33] to ensure isotropy. In the derivations to follow, it will be found that this is indeed the case.

[6] For a compressible fluid, Schlichting [33] has shown this improbability by considering the case of an isothermal sphere of gas subjected to uniform normal stress (no shear). If q, as defined in Eq. (34) is not invoked, the gas will undergo improbable *oscillations*.

[7] With reference to Fig. 1, evaluations in discretised space according to Eq. (38) will imply

$$(\bar{p}_{x_1})_P = \frac{\Delta x_{1e}p_W + \Delta x_{1w}p_E}{\Delta x_{1e} + \Delta x_{1w}} \quad (\bar{p}_{x_2})_P = \frac{\Delta x_{2n}p_S + \Delta x_{2s}p_N}{\Delta x_{2s} + \Delta x_{2s}}$$

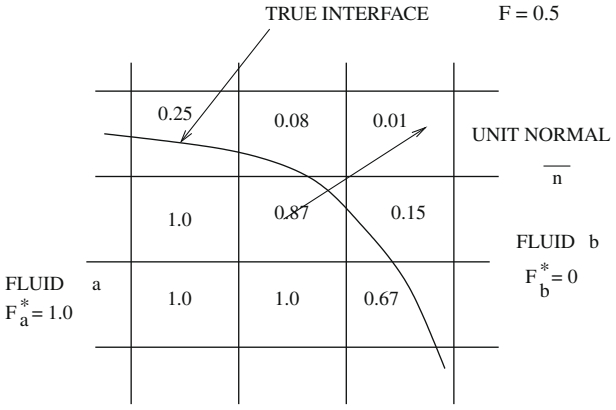

Fig. 2. *F*-Distribution and interface normal.

2.6. Evaluation of F_{st}

The surface tension force vector $\vec{F}_{st}$ acts *normal* to the interface. When surface tension coefficient σ is constant, the force per unit area is given by

$$\frac{\vec{F}_{st}}{A_{int}} = \sigma\kappa\vec{n} \tag{39}$$

where A_{int} is the interfacial area, $\vec{n}$ is the unit outward normal to the interface, κ is curvature of the interface (see Fig. 2) and,

$$\vec{n} = \frac{\nabla F}{A} \text{ with } A = \sqrt{\left(\frac{\partial F}{\partial x_1}\right)^2 + \left(\frac{\partial F}{\partial x_2}\right)^2 + \left(\frac{\partial F}{\partial x_3}\right)^2} \tag{40}$$

$$\kappa = \nabla\cdot\vec{n} = \frac{\partial n_{xi}}{\partial x_i} \tag{41}$$

Thus, the component of the force per unit volume in direction i (see Eq. (4)) is given by[8]

$$F_{st,i} = -\sigma\kappa\nabla F = -\sigma\kappa\frac{\partial F}{\partial x_i} = -\sigma\frac{\partial n_{xi}}{\partial x_i}\frac{\partial F^*}{\partial x_i} \tag{42}$$

where F^* is given by

$$F^* = 0.5\left\{1 + \frac{(F-0.5)}{|F-0.5|}\right\} \tag{43}$$

This replacement of F by F^* in Eq. (42) ensures that the surface tension force is evaluated at the interface (F=0.5) only even when F-distribution is smeared. Of course, $F^*_b = 0$ and $F^*_a = 1$. The main task now is to evaluate the curvature κ.

2.6.1. Geometric evaluation of κ

Most authors using VOF or Level-Set methods evaluate κ from Eq. (41) after *geometric reconstruction* of the interface. Thus, from Eq. (41),

$$\kappa = -\frac{1}{A}\left[\frac{1}{A}\frac{\partial F}{\partial x_i}\frac{\partial A}{\partial x_i} - \frac{\partial^2 F}{\partial x_i^2}\right] \text{ summation} \tag{44}$$

Following comments are now considered pertinent.

1. Evaluation of κ according to Eq. (44) is complex and is known to introduce discretisation errors. This has been shown by Takahira et al. [16] where a computation of a static bubble surrounded by static liquid generates spurious velocities.
2. Further, it is important to point out that many authors [23,17,18] study effect of surface tension coefficient σ by keeping the density and viscosity values of two fluids unchanged. As such, $F_{st,i}$ calculated using Eq. (44) produces different magnitudes of the force (see Eq. (42)) for the same fluid pair. However, in the literature, no real two fluid pairs having same values of density and viscosity but different values of σ are found. In our opinion such studies of effect of σ are misleading and are only of academic interest.
3. We believe that the source of the difficulty mentioned above can be traced to non-dimensionalisation of momentum Eq. (4). Many authors (see, [16], for example) use reference velocity U, reference length L and reference properties ρ_a and μ_a to non-dimensionalise Eq. (4). The dimensionless equation then reads

$$\frac{\partial\rho^*_m u^*_i}{\partial t^*} + \frac{\partial\rho^*_m u^*_j u^*_i}{\partial x^*_j} = \frac{1}{Re}\frac{\partial}{\partial x^*_j}\left[\mu^*_m\frac{\partial u^*_i}{\partial x^*_j}\right] - \frac{\partial p^*}{\partial x^*_i} + \rho^*_m g^*_i - \frac{\kappa^*}{We}\frac{\partial F^*}{\partial x^*_i} + \frac{1}{Re}\frac{\partial}{\partial x^*_j}\left[\mu^*_m\frac{\partial u^*_j}{\partial x^*_i}\right] \tag{45}$$

where the dimensionless terms are

$$Re = \frac{\rho_a U L}{\mu_a} \text{ Reynolds number} \tag{46}$$

$$g^* = \frac{gL}{U^2} \text{ Froude number} \tag{47}$$

$$\kappa^* = \kappa L \text{ Dimensionless curvature} \tag{48}$$

$$We = \frac{\rho_a U^2 L}{\sigma} \text{ Weber number} \tag{49}$$

$$\rho^*_m, \mu^*_m = \frac{\rho_m}{\rho_a}, \frac{\mu_m}{\mu_a} \text{ Dimensionless properties} \tag{50}$$

$$u^*_i, p^* = \frac{u_i}{U}, \frac{p}{\rho_a U^2} \text{ Dimensionless velocity and pressure} \tag{51}$$

$$x^*_i, t^* = \frac{x_i}{L}, \frac{t}{L/U} \text{ Dimensionless coordinates and time} \tag{52}$$

Eq. (45) thus shows that since κ^* is evaluated geometrically from F-distribution, the Weber number (We) now *appears* to be an *independent parameter* of the flow system. This, interpretation leads to investigation of effect of surface tension coefficient σ (or, We) for the same fluid pair. In the discussion below, we show that this is misleading and that Weber number is not an independent parameter of the flow system. Incidentally, in the literature, the Froude number is also defined as $\mathrm{Fr} = U^2/(gL)$.

2.6.2. Fluid dynamic evaluation of κ

In view of the last comment, we consider an alternative approach to evaluation of κ and $F_{st,i}$. Thus, we assume that the interface is a surface of *zero thickness having no physical properties*. Then, taking the dot-product of momentum Eq. (4) (along with Eq. (42)) with interface normal $\vec{n}$ will result in

$$\frac{\partial}{\partial n}(p - \tau_{nn}) = -\sigma\kappa\frac{\partial F^*}{\partial n} \quad \tau_{nn} = 2\mu\frac{\partial V_n}{\partial n} \tag{53}$$

where V_n is the velocity normal to the interface. Note that the unsteady, convective and gravity terms disappear because the interface has zero thickness and no mass. However, invoking the Stokes's requirement (with q = 0 for a control-volume of zero thickness normal to the interface)

$$p - \tau_{nn} = \bar{p} = -\sigma_n \tag{54}$$

Hence, Eq. (53) will read as

[8] Following thermodynamics convention, the negative sign acknowledges that the surface tension force is exerted *on the fluid*.

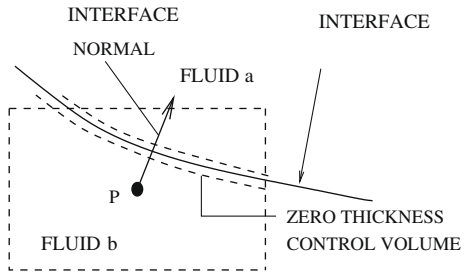

Fig. 3. Zero-thickness control volume surrounding an interface.

$$\frac{d\bar{p}}{dn} = -\sigma\kappa\frac{dF^*}{dn} \tag{55}$$

This equation is same as the familiar Young-Laplace equation for the equilibrium of a static bubble in a static fluid in which $\tau_{nn} = 0$ [42]. Here, τ_{nn} is finite. Now, upon discretisation (see Fig. 3) along the normal to the interface, it follows that

$$\sigma\kappa = -\frac{d\bar{p}/dn}{dF^*/dn} = -\frac{\bar{p}_b - \bar{p}_a}{F_b^* - F_a^*} = -\frac{\bar{p}_b - \bar{p}_a}{0-1} = \bar{p}_b - \bar{p}_a \tag{56}$$

and hence,

$$F_{st,i} = -(\bar{p}_b - \bar{p}_a)\frac{\partial F}{\partial x_i} \tag{57}$$

Following comments are now pertinent.

1. The remarkable feature of Eq. (57) is that evaluation of the surface tension force does not require value of σ at all. This is because, in Eq. (56) product $\sigma\kappa$ is directly evaluated as the difference of average pressures on either sides of the interface.[9]
2. On both structured and unstructured grids, the difference of average pressures can be evaluated following Eq. (37) as

$$\sigma\kappa = (\bar{p}_b - \bar{p}_a)_P = \frac{1}{3}(\bar{p}_b - \bar{p}_a)_{x_i,P} \text{ summation} \tag{58}$$

$$(\bar{p}_b - \bar{p}_a)_{x_i,P} = \text{ solution of } \frac{\partial^2}{\partial x_i^2}[p(1-2F^*)]_P = 0 \tag{59}$$

   This manner of evaluation ensures that $\sigma\kappa$ is calculated at the interface ($F = 0.5$) only.
3. *The interface shape is thus influenced by fluid properties $\rho_{a,b}$ and $\mu_{a,b}$ and the boundary conditions only which in turn determine the pressure and F distributions.*
4. This result may appear at variance with most previous researches but certainly accords with the practical fact that the same fluid pair cannot have different values of σ and hence, σ (or Weber number) is not an independent parameter of the flow system. In view of this variance with previous researches, in the companion paper [43], we have computed two problems with both geometric and fluid dynamic evaluations of $F_{st,i}$ and compared the interface evolutions. Of course, the ultimate validity of the fluid dynamic as well as geometric evaluation of the surface tension force can only emerge from comparison with experiment. Unfortunately, we do not have access to any experimental data to demonstrate merits of either evaluations.

[9] It is appropriate to mention that Sussnman et al. [14] do recognise the validity of Eqs. 54 and 56 but they do not use them to evaluate the surface tension force as done here.

3. Conclusions

1. In this paper the problem of prediction of unsteady flow of two immiscible incompressible fluids is formulated within the single fluid formalism. Discretised Navier–Stokes equations are solved on collocated grids after invoking the requirement of Stokes's laws for an isotropic fluid.
2. Equations are solved in a fully-implicit manner at each time step by adapting the computer code given in [28]. The overall calculation procedure is also applicable to three-dimensional unstructured meshes [31].
3. The VOF and Conserved-Scalar equations are derived from the mass-conservation equation with an intent to serve a pedagogic purpose.
4. The satisfaction of requirement Stokes's stress–strain relations leads to
   (a) Alleviation of the problem of zig-zag pressure prediction as well as the problem of loss of volume/mass during unsteady computations over large times.
   (b) Fluid-dynamic interpretation of interface curvature which in turn evaluates the surface tension force without requiring knowledge of surface tension coefficient σ.
5. The fluid dynamic interpretation of the surface tension force shows that the Weber number cannot be an independent parameter of the flow system. This is at variance with the interpretation that is routinely associated with the geometric evaluation of interface curvature in all previous publications.
6. TVD scheme is used for representation of convective terms to reduce interface smearing.

The companion paper [43] shows application of the method developed in this paper.

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