AN IMPLICIT ALGORITHM FOR CAPTURING SHARP FLUID INTERFACES IN THE VOLUME OF FLUID ADVECTION METHOD

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Abstract. The Volume of Fluid (VOF) method is one of the most effective methods employed in the simulation of two fluid flows with interfaces where density and viscosity change abruptly. These interfaces are represented implicitly by the values of a colour function which is a volume fraction of one of the fluids. The advantage of the method is its ability to deal with arbitrarily shaped interfaces and to cope with large deformations, as well as interface rupture and coalescence in a natural way. In comparison to a level set method, the mass is rigorously conserved in VOF, provided the discretisation is conservative, but one of the main difficulties is advecting the interface without diffusing, dispersing, or wrinkling it. This can either be performed algebraically, in schemes such as CICSAM or geometrically, in schemes such as PLIC.

In the present paper, an algebraic advection scheme for the interface is presented, which is designed for the implicit time advancing algorithm. Analogous to CICSAM, the new scheme switches smoothly between ULTIMATE-QUICK and the upper bound of the universal limiter, depending on the angle between the interface and the flow direction. Four cases are tested with the present scheme: (i) solid body rotation; (ii) circle in a shear flow; (iii) dam-break and (iv) Rayleigh-Taylor instability. In the first two test cases, prescribed velocity fields are used, thereby allowing the effectiveness of the scheme in advecting the colour function only to be assessed. The scheme is found to outperform six other methods used for comparison in both studies. In solid body rotation simulations a fractional error of 0.19% is calculated in comparison to the next best recorded error of 1.1%. Similarly, in the longest shear flow simulation, a fractional error of 1.2% is calculated in comparison to the next best recorded error of 3.9%. In the final two test cases the advection equation for the colour function is coupled to the Navier-Stokes equations. In dam-break simulations it is found that the resulting solution effectively captures the trends displayed in experimental data for the advancing water front and the residual height of the liquid column against time. Qualitative results obtained for the Rayleigh-Taylor instability modelling in test case four are found to compare favourably to previous numerical simulations of the same phenomenon.

1 INTRODUCTION

The accurate numerical computation of multi-fluid flows and the simulation of the flow of two immiscible fluids separated by a well-defined interface, has many applications. One area is that of environmental engineering where it is used to simulate dam and dyke-breaks¹, volcanic flows and plumes² and the motion of water in a marine environment.³ Another is that of biomedical sciences/engineering, where biological material and fluids such as blood are transported through capillary tubing and channels in the vascular system⁴ or in Micro Electro Mechanical Systems (MEMS) devices.⁵

Current numerical methods for simulating such two-phase flows with discrete interfaces can be generally classified as either *interface-tracking (surface) methods* or *interface-capturing (volume) methods*.⁶ In *interface-tracking methods* the free surface is treated as a sharp interface whose motion is followed. These methods are often implemented through the use of *moving grid techniques*⁷ or *height functions*.⁸ Whilst surface methods maintain a sharp interface whose exact position is known throughout the calculation, they require special treatment when the interface is subject to large deformation or stretching.⁹ Conversely, *interface-capturing methods* cope well with large stretching and deformation of the interface as well as rupture and coalescence. Their implementations include massless particles¹⁰ or the use of an indicator function.

In the second approach, the indicator function is usually a scalar step function (known as a colour function) representing the volume fraction of space occupied by one of the fluids (known as VOF¹¹), or a smooth but arbitrary function (level set¹²) encompassing a predefined iso-surface which identifies the interface. The advantage of this method is that conservation can be enforced, since a scalar transport equation is solved in an Eulerian manner, but one of the main difficulties is advecting the step function without diffusing, dispersing or wrinkling the interface. Various techniques have been proposed for capturing a well-defined interface using volume fractions and these are based largely on either a geometric or algebraic approach. In the geometric approach¹³, volume fractions (that are moved and updated by the velocity field) are used to construct line segments across cells, providing a geometrical form of the interface. A major problem with such methods is that the cell shapes are implicitly used in the interface reconstruction and so it is very difficult to extend these techniques to arbitrary complex meshes and to three dimensions.

Alternatively an algebraic approach can be adopted in which the convective scalar transport equation for the volume fraction is discretised in such as way so as to guarantee physical (bounded) volume fractions whilst preventing smearing of the interface over several mesh cells. A problem with the original VOF¹¹ method is that it does not preserve local boundedness i.e. a volume fraction value which initially lies between the values of its neighbours does not necessarily preserve this property when advected in the absence of shear. This numerically introduces new maxima and minima into the volume fraction field and leads to non-physical deformation of the interface shape.¹⁴⁻¹⁷

High resolution differencing schemes such as Total Variation Diminishing (TVD) methods, Flux Corrected Transport (FCT) schemes and techniques using Normalised Variable Diagrams (NVD)¹⁸ offer another approach, but attempts to apply them show that they are too

diffusive.^{19, 20} Although FCT schemes are non-diffusive by nature they create areas of unphysical flotsam (floating wreckage) or jetsam (jettisoned goods).¹⁵ Furthermore these schemes are based on one-dimensional derivations with extensions to multi-dimensional flow by operator splitting.²¹ This limits their implementation to structured meshes whose control volume faces are aligned with the coordinate axes.

Ubbink & Issa²² have presented an algebraic advection scheme known as the Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM). This makes use of the NVD concept and switches between differencing schemes to yield a bounded scalar field, but one which preserves both the smoothness of the interface and its sharp definition (over one or two computational cells). This paper presents an implementation of CICSAM for the implicit time advancing algorithm and assesses its performance in a number of test cases.

2 GOVERNING HYDRODYNAMIC EQUATIONS

In the VOF method, a one fluid formulation of two-fluid Navier-Stokes equations is employed as the interfacial boundary conditions are implicitly contained in the equation of motion. Both fluids are described by the same set of equations, but the differences in material properties, such as density and viscosity, are explicitly accounted for. Consider two incompressible fluids, 1 and 2, separated by an interface S. The continuity equation is given by:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

where u_i is the velocity and x_i is the spatial direction. The flow is governed by the incompressible Navier-Stokes equations:

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_j u_i}{\partial x_i} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{1}{\rho} \frac{\partial \tau_{ij}}{\partial x_i} + \frac{F_i}{\rho} + g_i$$
(2)

in which *p*, g_i and F_i are the pressure, gravity vector and the interfacial surface tension force, respectively and τ_{ii} is the viscous stress tensor given by:

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}$$
(3)

where μ is the coefficient of dynamic viscosity and δ_{ij} is the Kronecker delta. The local density ρ and viscosity μ are defined as:

$$\rho = C\rho_1 + (1 - C)\rho_2 \text{ and } \mu = C\mu_1 + (1 - C)\mu_2 \tag{4}$$

where the subscripts denote the different fluids and C is the volume fraction with a value of unity in fluid 1 and zero in fluid 2. The volume fraction is governed by:

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = 0 \tag{5}$$

The Continuum Surface Force (CSF) model of Brackbill *et al.*²³ has been frequently employed to calculate the surface tension force and is given by:

$$F_i = \sigma \kappa \frac{\partial C}{\partial x_i} \tag{6}$$

where σ is the surface tension and κ is the curvature of the interface. The CSF method converts the surface force into a volumetric continuous force, F_i , instead of a boundary condition on the interface. Equations (1)-(6) are discretised using a finite-volume method and an implicit temporal scheme. The pressure and velocity fields are solved on a collocated grid using the SIMPLE²⁴ algorithm coupled through Rhie and Chow interpolation.²⁵ Eq. (5) is essential for capturing the motion of the fluid interface but accurate discretisation of its steplike behaviour is not straightforward and is the focus for the remainder of the paper.

The method of solution operates in an iterative fashion, wherein the equation for the colour function, Eq. (5), is solved first (starting from an initial volume field) and the resultant volume fractions are used to compute the new densities and viscosities throughout the domain according to Eq. (4). The momentum and continuity equations are solved utilising these new values and the process repeats through a number of outer iterations until a suitable convergence criterion has been satisfied, for each time step.

3 DESCRIPTION OF THE SCHEME

3.1 Discretisation of the equation

Consider the integral form of Eq. (5) over each control volume and time interval Δt . Then a finite-volume first order implicit discretisation gives:

$$C_P^{t+\Delta t} = C_P^t - \frac{\Delta t}{V_P} \sum_f (C_f F_f)^{t+\Delta t}$$
(7)

where *P* denotes the centre of the control volume (with volume V_P), *f* is the centroid of the cell face, the volumetric flux is given by the term $F_f = \mathbf{A}_f \cdot \mathbf{u}_f$ where **A** is the outward-pointing face area vector normal to the face and the summation is over all cell faces.

For a cell-centred method, such as that which we will be considering, the cell centre values are used to interpolate the values of the colour function on the faces C_f in Eq. (7). Figure 1 contains a schematic representation of a one-dimensional control volume. The centre cell (donor cell), referred to with subscript D, has two nearest neighbours, referred to with subscripts A for the acceptor cell and U for the upwind cell. Note that the flow direction determines the location of the neighbours. The face between the donor and acceptor cell with subscript *f* is the face under consideration.



Figure 1: One dimensional control volume

Linear interpolation of the face value, known as central differencing, is second order accurate but results in an unbounded solution for problems in which convection dominates. The use of the donor cell value (upwind differencing) guarantees a bounded solution but is diffusive and smears the transitional area between the fluids over several cells. The use of the acceptor cell value (downwind differencing) does not preserve boundedness but maintains resolution of the interface. Hence the problem of interface tracking boils down to the selection of a combination of differencing schemes which will preserve both the boundedness of the volume fraction distribution and the sharpness of the interface. To overcome this problem Ubbink & Issa²² proposed that the switch should be between

To overcome this problem Ubbink & Issa²² proposed that the switch should be between two high-resolution schemes which comply with local boundedness criteria. They argued that a bounded compressive scheme should be used when the interface orientation is more likely to be normal to the flow direction and that a more accurate interpolation scheme, such as bounded central differencing or bounded quadratic upwind interpolation, should be used when the interface is more likely to be tangential to the direction of motion. Furthermore they have demonstrated that the switch between schemes should be more gradual, rather than the sudden switch proposed by the original VOF scheme. Their mechanism for switching and the highresolution schemes employed, are described next.

3.2 Normalised Variable Diagram (NVD)

The normalised variable, as proposed by Leonard,¹⁸ forms the basis on which the high resolution schemes are constructed and is defined as:

$$\tilde{C} = \frac{C - C_U}{C_A - C_U} \tag{8}$$

The normalised variable can be used to give expressions for $\tilde{C}_{_D}$ and $\tilde{C}_{_f}$:

$$\tilde{C}_{_{D}} = \frac{C_{_{D}} - C_{_{U}}}{C_{_{A}} - C_{_{U}}} \text{ and } \tilde{C}_{_{f}} = \frac{C_{_{f}} - C_{_{U}}}{C_{_{A}} - C_{_{U}}}$$
(9)

Gaskell & Lau²⁶ have presented a convection boundedness criterion (CBC) for onedimensional implicit flow calculations. The CBC uses the normalised variable and stipulates bounds on \tilde{C}_{f} for which an implicit differencing scheme in 1D will always preserve the local boundedness criteria:

$$\begin{cases} \tilde{C}_{f} = \tilde{C}_{D} & \text{for } \tilde{C}_{D} < 0 \text{ or } \tilde{C}_{D} > 1 \\ \tilde{C}_{D} \leq \tilde{C}_{f} \leq 1 & \text{for } 0 \leq \tilde{C}_{D} \leq 1 \end{cases}$$
(10)

Leonard¹⁸ has shown that various difference schemes and the CBC can be reconstructed for one-dimensional transitional flow calculations using a linear weighting based on the Courant number α , given as:

$$\tilde{C}_{f} = (1 - \alpha)\tilde{C}_{f}^{*} + \alpha\tilde{C}_{D}$$
(11)

where \tilde{C}_{f}^{*} is the normalised face value for the implicit implementation. With this linearisation $\tilde{C}_{f} \rightarrow \tilde{C}_{f}^{*}$ if $\alpha \rightarrow 0$ and $\tilde{C}_{f} \rightarrow \tilde{C}_{D}^{*}$ if $\alpha \rightarrow 1$; thus a point to point transfer of the upwind nodal value occurs if $\alpha_{f} = 1$. For transitional flow calculations, the CBC reduces to the universal limiter¹⁸ given by:

$$\begin{cases} \tilde{C}_{f} = \tilde{C}_{D} & \text{for } \tilde{C}_{D} < 0 \text{ or } \tilde{C}_{D} > 1 \\ \tilde{C}_{D} \leq \tilde{C}_{f} \leq \min\left\{1, \frac{\tilde{C}_{D}}{\alpha}\right\} & \text{for } 0 \leq \tilde{C}_{D} \leq 1 \end{cases}$$
(12)

Figure 2(a) shows the NVD region for this transitional flow implementation with an arbitrary Courant number $\alpha = 0.2$.

A differencing scheme which follows the upper bound of the universal limiter for transitional flow calculations is shown to be very compressive because it turns every finite gradient in a scalar field into a step profile.¹⁸ Named as HYPER-C by Leonard¹⁸ it is precisely the scheme required when the interface is more likely to be normal to the flow direction.

Although the upper bound of universal limiter as defined in Eq. (12) was derived for explicit schemes it can be seen that its bounded region is merely a subset of the full region defined in Eq. (10) for implicit schemes. The current implicit scheme can therefore utilise this more restrictive criterion, because it guarantees boundedness and provides a compressive scheme to use in appropriate situations where the interface is more normal to the direction of motion. This knowledge was applied by Ubbink & Issa to generate CICSAM,²² the basis of the current scheme described in the next section.

3.3 Basis of CICSAM and the current implicit scheme

As has already been stated, the HYPER-C scheme is the most suitable for the advection of a step profile when the interface is normal to the flow direction. The original VOF scheme¹¹ determines the slope of the interface and switches to upwind differencing if the smallest angle between the interface and the face of the control volume is greater than 45°. An extensive study conducted by Lafaurie *et al*,¹⁶ highlighted extensive problems with such an abrupt switching. Ubbink & Issa²² proposed two main changes. Firstly the scheme should concentrate on how to switch and not when to switch and secondly that some other higher order scheme, other than upwind differencing should be used. Their CICSAM scheme employed ULTIMATE-QUICKEST¹⁸ in this role, but in the spirit of Leonard's ULTIMATE¹⁸

strategy, the current scheme employs ULTIMATE-QUICK, a combination of the universal limiter and QUICK.²⁷ The mathematical formulation of ULTIMATE-QUICK in the NVD is:

$$\tilde{C}_{f_{\text{UQUKK}}} = \begin{cases} \min\left(\frac{6C_D + 3}{8}, \tilde{C}_{f_{\text{UL}}}\right) & \text{when } 0 \le \tilde{C}_D \le 1\\ \tilde{C}_D & \text{when } \tilde{C}_D < 0, \tilde{C}_D > 1 \end{cases}$$
(13)

Ubbink & Issa²² defined a weighting factor $0 \le \gamma_f \le 1$ based on the angle between the interface and the direction of motion to calculate the normalised face value. This weighting factor ensures a smooth transition between the upper bound of the universal limiter given by Eq. (12) and the less compressive differencing scheme, represented by ULTIMATE-QUICK, given by Eq. (13). The face value is defined as:

$$\tilde{C}_{f} = \gamma_{f} \tilde{C}_{f_{\text{UL}}} + \left(1 - \gamma_{f}\right) \tilde{C}_{f_{\text{UQUICK}}}$$
(14)

where $\gamma_f = 1$ is used when the interface is normal to the direction of motion and $\gamma_f = 0$ is used when the interface is tangential to it. As described by Ubbink & Issa,²² this implies that ULTIMTE-QUICK operates where the universal limiter fails to preserve the gradient in the interface and that the universal limiter operates where ULTIMATE-QUICK fails to maintain the sharpness of the interface. The basic derivation of the scheme is complete by stating Ubbink's & Issa's²² definition of the weighting factor γ_f . This is based on the cosine of the angle θ_f between $(\nabla C)_D$, the vector normal to the interface and the vector \mathbf{d}_f which connects the centres of the donor and acceptor cells and is given by:

$$\gamma_f = \min\left(k_\gamma \frac{\cos(2\theta_f) + 1}{2}, 1\right) \tag{15}$$

where:

$$\theta_{f} = \cos^{-1} \left| \frac{(\nabla C)_{D} \cdot \mathbf{d}_{f}}{\left| (\nabla C)_{D} \right| \left| \mathbf{d}_{f} \right|} \right|$$
(16)

and $k_{\gamma} \ge 0$ is a constant introduced to control the dominance of the different schemes (recommended value of $k_{\gamma} = 1$). The NVD for the scheme is shown in Figure 2(b).

Although the normalised face value, predicted with the current differencing scheme for one-dimensional uniform flow, in Eq. (14) is important, the actual face value can be derived by algebraic manipulation of Eq. (9) to give:

$$C_f = (1 - \beta_f)C_D + \beta_f C_A \tag{17}$$

where:

$$\beta_f = \frac{\tilde{C}_f - \tilde{C}_D}{1 - \tilde{C}_D} \tag{18}$$



Figure 2: (a) The universal limiter for explicit flow schemes, at an arbitrary Courant number value of 0.2 and (b) NVD for the implicit differencing scheme as defined by the universal limiter and ULTIMATE-QUICK

The weighting factor β_{f} , which implicitly contains the upwind value C_{U} (in the definition of the normalised variables), carries all the information regarding the fluid distribution in the donor, acceptor and upwind cells as well as the interface orientation relative to the direction of motion.

In accordance with CICSAM,²² it can be seen from the NVD in Figure 2(b) that the formal order of accuracy is not uniform. It varies from first order (upwind or downwind) to second order (centred) to even third order (QUICK) depending on the approximation used for the surface integral over the face.

4 SIMPLE ADVECTION TESTS

Initial problems for the scheme were chosen so as to test the advection of the colour function alone. To this end, analytic velocity fields were used and no attempt was made to couple the advection of C to solutions of the Navier-Stokes equations.

4.1 Simulation of Zalesak's rotating solid body problem

One such test is the "solid body" problem as described by Zalesak.²⁸ This problem specifically tests the ability of the scheme to translate and rotate a fixed volume, as the fluid region should not deform during the advection.

A uniform 2-D square mesh of grid size 200×200 cells was employed to represent a square domain of side 4.0 in length. A slotted circle was created by removing a slot of width 0.12, from a circle of radius 0.5 and a finite boundary of half the grid spacing was placed around the entire structure. Initially the fraction of fluid within a cell, $C_{i,j}$ at position (i, j) was set to zero inside the structure and unity outside. Values in the boundary were given by linear interpolation, perpendicular to straight edges and radially at the corners and on the curved edge.

The structure was subject to a unidirectional velocity field, whose components were given by:

$$u = -\Omega(y - y_0), v = \Omega(x - x_0)$$
 (19)

where $(x_0, y_0) = (2.0, 2.0)$ is the centre of rotation and where Ω is the angular velocity of 0.5 rads/s. The circle's geometric centre was located at the point (x, y) = (2.0, 2.75), with 2524 time steps used for one full rotation. The fractional error *E* resulting from the simulation was calculated using:

$$E = \frac{\sum_{i,j} \left\| C_{i,j}^{end} - C_{i,j}^{0} \right\|}{\sum_{i,j} C_{i,j}^{0}}$$
(20)

where C^{end} is the solution (for the fraction of fluid) at the end of the simulation, C^0 is the initial solution and the summation takes place over all cells at position (i, j).

4.1.1 Numerical results

Figures 3(a)-(b) show the shape of the slotted circle at the beginning and end of the simulation for one full rotation. Qualitatively, the results displayed in Figure 3 compare favourably to those obtained by Rudman¹⁵ and Ubbink & Issa.²² It is found that advecting the discontinuities present at the corners poses the greatest difficulty for the scheme.



Figure 3: Results for solid body rotation, illustrating the fraction of fluid C through the domain as denoted by the colour scheme in each legend. a) The initial configuration; b) after one full revolution.

The calculated fractional error, as defined in Eq. (20), is displayed in Figure 4(a), together with those obtained for six other methods.^{15, 22} As can be seen from Figure 4(a), the error associated with the present scheme is approximately an order of magnitude less than those previously obtained. This may be attributable to the implicit nature of the present algorithm, which advances the interface with the same up-to-date flow information in all coordinate directions. The results obtained for the fractional error against increasing time of simulation are displayed in Figure 4(b). It can be seen that even after four full rotations, the fractional error accumulated by the present scheme has reached a value of 0.006. This is still lower than



the value of 0.0109 that was calculated for the next best scheme (Youngs) after only one rotation.

Figure 4: (a) Errors obtained after one full rotation of the slotted circle for the current scheme (THOR) and six other methods^{15, 22} and (b) the fractional error measured against time (in units of full rotations).

4.2 Simulation of the shearing flow problem in two dimensions

An additional and arguably more demanding problem is the shearing flow simulation, as described by Rudman¹⁵ and Ubbink & Issa.²² The introduction of a shear in the velocity field ensures that topological change occurs as the fluid volume is deformed.

A square mesh, consisting of 100×100 uniform cells, was used to represent a square domain of side π in length. A circle of radius 0.2π with a finite boundary of width half the grid spacing was centred at position $(0.5\pi, 0.2(1+\pi))$. Initially the fraction of fluid within each cell, $C_{i,j}$ at position (i, j) was set to zero inside the circle and unity outside, with values in the boundary given by linear interpolation in the radial direction. The shearing velocity field was given by components:

$$u(x, y) = \cos(x)\sin(y) , \quad v(x, y) = -\sin(x)\cos(y)$$
(21)

where $|\mathbf{V}|_{\text{max}}$, the maximum magnitude of the velocity field on the domain, has the value of $\sqrt{2}$ in the corners of the domain as both components are unity. Thus at the corners of the domain the requirement is that:

$$\Delta t \le \frac{\sqrt{\Delta x^2 + \Delta y^2}}{\left|\mathbf{V}\right|_{\max}} = \frac{\sqrt{2\Delta}}{\left|\mathbf{V}\right|_{\max}}$$
(22)

This was obtained by enforcing the condition that the speed of information propagation on the domain should not exceed the fluid velocity. Since the maximum Courant number must be less than unity, it follows from Eq. (22) that:

$$c_{\max} = \frac{|\mathbf{V}|_{\max} \,\Delta t}{\sqrt{2\Delta}} \tag{23}$$

From the comparison studies,^{15, 22} it was clear that a maximum Courant number of 0.25 had been used throughout the simulations. Using Eq. (23), a value of $\Delta t = \pi/400$ was calculated and used in order to fairly compare the results. Each simulation ran for *N* time steps, before reversing the sign of the velocity field and integrating for another *N* time steps, in an attempt to recover the initial configuration. Values of *N* in the range $250 \le N \le 2000$ were tested.

A study of the effect of the Courant number on the fractional error *E* given by Eq. (20), was also completed over simulations of equal duration. In this case a mid-way time of 7.854s was chosen, prior to reversing the sign of the velocity field and integrating for the same period again. The Courant number was varied by changing both the time step and grid spacing and results were obtained in the range $0.25 \le c_{max} \le 1.25$.

4.2.1 Numerical results

Results for the fraction of fluid at three stages during the simulations for N = 1000 and N = 2000 are shown in Figures 5(a)-(f).



Figure 5: Surface plots of the value of the fraction of fluid for a) initial configuration prior to integration b) after integrating forward 1000 steps c) after integrating back for another 1000 and d) initial configuration prior to integration e) after integrating forward 2000 steps f) after integrating back for another 2000.

The illustrations in Figure 5 compare favourably to those presented in references 15 & 22. It can be seen that as the shearing field stretches the circle, the scheme struggles to capture the tail which is perhaps only 1-2 grid cells in size. The remnants of the tail are clearly visible in

the bottom left of the circle in Figures 5(c) & 5(f) and this has an increasingly larger effect on the calculated fractional error as the integration time increases.

Results for the error *E* after *N* time steps (forward and back) are shown in Figure 6(a) for each of the methods described^{15, 22} and for the current scheme (marked THOR). It can be seen from the calculated errors in Figure 6(a) that the current scheme outperforms those given in references 15 & 22.



Figure 6: (a) The fractional error E against N for each of the schemes as indicated in the legend and (b) Fractional errors obtained during repeats of the N=1000 simulation for a range of maximum Courant numbers

Results for the value of the fractional error E against maximum Courant number are shown in Figure 6(b). These simulations were performed over a set time, in each case 7.854s. Initially the grid remained unchanged and the time step was systematically increased in order to vary the Courant number, providing the results labelled "Time" in Figure 6(b). After this, a fixed time step was employed and a number of different grids of increasing resolution were employed to vary the Courant number. The results of these simulations are labelled "Space" in Figure 6(b). Note that the Courant numbers quoted are the maximum values found on the domain during that simulation.

5 SIMULATION OF THE COLLAPSE OF A LIQUID COLUMN IN TWO DIMENSIONS

5.1 Overview of the numerical simulation

A number of problems, incorporating coupling of the advection of the colour function with solutions to the momentum equations were then solved. One such problem is the collapse of a liquid column (e.g. a dam-break) for which experimental data is available for comparison. The principle source used in this study was the paper of Martin & Moyce,²⁹ which describes an experimental investigation of this problem and contains experimental measurements. The paper by Kim & Lee⁷ also describes a numerical simulation of this problem and was used as an initial starting point to setup the problem and later as a useful reference for comparison.

The separate collapses of two liquid columns in two dimensions were studied. The first was that of a square column of side 0.05715m and the second a rectangular column of height 0.1143m, width 0.05715m. Numerical integration was carried out over a total simulation time of 0.13s and 0.23s for the square and rectangular columns respectively.

5.2 Experimental procedure

In the first test case, that of the square column, four separate grids were employed and both a fixed and variable time step were used. Table 1 shows the key spatial and temporal parameters used in each simulation. An additional simulation was also run on each grid. This used a variable time step whose value was recalculated as the simulation progressed in order to maintain a constant maximum Courant number of 0.1.

Physical Grid Size, horizontally and vertically (m)	Grid Size in units of Column Height , H,	Cells used in the horizontal (x) and vertical (y)	Horizontal Grid Step Δx (m)	Vertical Grid Step Δy (m)	Time Step, when used Δt (s)
	and vertically	directions			
0.2286 x 0.06858	4H x 1.2H	64 x 19	3.57×10 ⁻³	3.61×10 ⁻³	2.0×10^{-4}
0.2286 x 0.06858	4H x 1.2H	80 x 24	2.86×10^{-3}	2.86×10^{-3}	2.0×10^{-4}
0.2286 x 0.06858	4H x 1.2H	160 x 48	1.43×10 ⁻³	1.43×10 ⁻³	1.0×10^{-4}
0.2286 x 0.06858	4H x 1.2H	320 x 96	7.14×10^{-4}	7.14×10^{-4}	1.0×10^{-4}

Table 1: The parameters used in each of the simulations for the square liquid column. Note that all dimensions are described horizontally and then vertically and that four additional simulations employing the same grid parameters but variable time steps were also completed.

In the second test case, that of the rectangular column, three separate grids were used and as above, both a fixed and variable time step were employed. Table 2 lists the grid and time step parameters used in each simulation.

Physical Grid Size, horizontally and vertically (m)	Grid Size in units of Column Height H	Cells used in the horizontal (x) and vertical (y)	Horizontal Grid Size Δx	Vertical Grid Size Δy	Time Step, when used Δt
(111)	horizontally	directions	(m)	(m)	(\$)
	and vertically				
0.4572 x 0.13716	4H x 1.2H	80 x 24	5.72×10 ⁻³	5.72×10 ⁻³	2.0×10^{-4}
0.4572 x 0.13716	4H x 1.2H	160 x 48	2.86×10^{-3}	2.86×10^{-3}	2.0×10^{-4}
0.4572 x 0.13716	4H x 1.2H	320 x 96	1.43×10^{-3}	1.43×10^{-3}	1.0×10^{-4}

Table 2: The parameters used in each of the simulations for the rectangular liquid column. Note that all dimensions are described horizontally and then vertically and that four additional simulations employing the same grid parameters but variable time steps were also completed.

In both test cases, the liquid column is initially in hydrostatic equilibrium and is "confined" between the left vertical wall of the grid and a notional gate. The fraction of fluid in a cell at position (i, j), represented $C_{i,j}$ is initially set to unity inside the water column, and zero outside, with a finite boundary of one grid cell being used on the surface. Values for the fraction of fluid inside the boundary are given by linear interpolation in the direction perpendicular to the boundary surface. The gate is suddenly removed at time $t = 0^+$ and the water column starts to collapse under the influence of gravity. Frictionless boundary conditions are specified on the bottom and vertical walls. The density and viscosity of water are taken as 1.0 kg/m^3 and $1.0 \times 10^{-3} \text{ kgm}^{-1}\text{s}^{-1}$ respectively. The ambient fluid is air. Density is taken as $g = 9.81 \text{ m/s}^2$.

5.3 Numerical results

Figure 7 illustrates a typical collapse in time, in this case that of a square column on the 160 x 48 grid using a fixed time step. An interesting feature of the simulation depicted in Figure 7 is the presence of a horizontal jet on the water front. Although these are not visible in photographs of the collapse shown in reference 29, such jets are present in similar experiments performed by Stansby, Chegini & Barnes¹ using modern imaging techniques and equipment. A close up of this feature for the example given in Figure 7 is shown at time t = 0.13 s in Figure 8.



Figure 7: The collapse of the square water column on the 160 x 48 grid using a fixed time step at each of the times shown. Each plot shows the fraction of fluid in each cell throughout the domain as given by the spectrum in the attached legend.

Figure 8 illustrates the velocity field profile in the vicinity of the jet. It can be seen that the low volume fraction region on top of the jet appears to be travelling more slowly, as in encounters resistance from the air in the domain. It is likely that this low volume fraction region is a mixed water-droplet/air spray. The effect continues just in front of and above this region where there is a general upward turning in the velocity field as the air is pushed up and over the jet and turns backs.



Figure 8: An expanded view of the horizontal jet feature. Velocity vectors are plotted, with relative lengths indicating the magnitude of the velocity at that point on the domain. Contours of 0.1, 0.5 and 0.9 are plotted in the volume fraction field.

The position of the water wave front and the height of the residual water column are plotted as functions of elapsed time and compared with experimental data.²⁹ Figures 9-10 show these plots for the square water column. It should be noted that these simulations correspond to the a = 2.25 inch and $n^2 = 1$ experiment of Martin & Moyce,²⁹ where *a* is the width of the liquid column and *n* is defined as a constant such that n^2a is the height of the column. All values have been rescaled to the appropriate dimensionless units described therein.

Horizontally, the distance travelled by the water front from its initial starting point is defined as *Z*, where Z = x/a. Vertically the quantity *H* represents the residual height, i.e. in comparison to the original starting state. This is defined by $H = y/(n^2 a)$. Time is defined in two separate units, dependent upon the direction of motion under consideration. Horizontally the unit is *T*, where $T = nt\sqrt{g/a}$ and vertically τ , where $\tau = t\sqrt{g/a}$.

Figures 9(a)-(b) show the position of the water front and residual column height against time for the simulations performed using a fixed time step for each of the four grids as described in Table 2, whilst Figures 10(a)-(b) show the position of the water front and residual column height against time, for the simulations run using a variable time step on each of the four grids described in Table 2.

It can be seen from Figures 9-10 that there is excellent agreement between the results obtained from numerical simulation and the experimental data. In particular, the general trends followed by the experimental data are clearly modelled in each of the simulations. It can be seen that the results obtained on the two finest grids in each case are very closely



matched, indicating that the grid spacing is sufficiently small to have reached a grid independent solution.

Figure 9: (a) The position of the water front and (b) the height of the residual water column against time for the square column using a fixed time step



Figure 10: (a) The position of the water front and (b) the height of the residual water column against time for the square column using a variable time step and a fixed maximum Courant number of 0.1.

Conversely it is also clear from the results for the residual column height that the coarsest grid has failed to accurately map the experimental trend in this case. The oscillatory nature of the graph (particularly evident for the 64 x 19 grid results in Figure 9(b)) is due to linear interpolation being used to locate the boundary surface on a very coarse grid.

A time lag between the numerical and experimental results, particularly evident in Figures 9(a) & 10(a), exists. This may be caused by the fact that experimentally it is very difficult to remove the gate instantaneously and thus there is a finite delay before the column begins to fully collapse. An average value of this delay was calculated by comparing experimental data points 3–8, where the solution is fully developed, to those obtained using the finest grid. The delay was found to be $T = (0.16 \pm 0.01)$ dimensionless units, corresponding to a real time of (12 ± 1) ms.

Figures 11-12 show the same results for the rectangular water column. It should be noted that these correspond to the $n^2 = 2$ and a = 2.25 inch experiment of Martin & Moyce²⁹ with values rescaled to the appropriate dimensionless units as already described. It should also be noted that the shortened graphs for the finest grid in Figures 11-12 are due to insufficient computing time being available to complete the simulations.



Figure 11: (a) The position of the advancing water front and (b) the residual height of the water column against time for the rectangular column using a fixed time step.



Figure 12: (a) The position of the advancing water front and (b) the residual height of the water column against time for the rectangular column, using a variable time step and a fixed maximum Courant number of 0.1.

Once again the trends displayed in the experimental and numerical data show excellent agreement. As described above, the finite delay between the numerical and experimental data is also clearly visible in these results. This time an average value for the delay was calculated by comparing experimental data points 4-11 against the solution for the finest grid. The delay was found to be approximately $T = (0.22 \pm 0.02)$ dimensionless units, corresponding to a real time of (12 ± 1) ms, which is identical to that calculated for the square liquid column.

6 RAYLEIGH-TAYLOR INSTABILITY MODELLING

6.1 Overview of Rayleigh-Taylor instability simulation and experimental procedure

The final problem investigated was that of the Rayleigh-Taylor instability, as presented by López *et al.*³⁰ A heavy fluid of density $\rho_1 = 1.225 \text{ kg/m}^3$ is placed above a lighter fluid of density $\rho_2 = 0.1694 \text{ kg/m}^3$ in a rectangular domain 1m wide by 4m high. The viscosity of both fluids was taken as $3.13 \times 10^{-3} \text{ kgm}^{-1}\text{s}^{-1}$. Due to the symmetry of the problem, only half of the physical domain was solved. This was represented by a grid of 32 x 256 cells in the horizontal and vertical directions respectively. The integration was performed using a

variable time step, but constant maximum Courant number of 0.1 in the domain, in order to reduce computing time. Free slip boundary conditions were imposed at both the upper and bottom boundaries, with both lateral boundaries having symmetry conditions imposed upon them. The interface shape was initially given by the cosine function $y = -0.05 \cos(2\pi x)$.

6.2 Numerical results for Rayleigh-Taylor instability modelling

Figure 13 shows the progression of the Rayleigh-Taylor instability simulation with time.



Figure 13: Illustration of the progression of the Rayleigh-Taylor instability with time as given by the fraction of fluid across the domain at each of the times shown.

As can be seen in Figure 13, the results are qualitatively comparable to those in reference 30 and the general form of the nonlinear dispersion of the more dense material, displays a similar pattern. Particular points of similarity are the downward vertical plume at the right edge of the domain, the upward hook emanating from the left edge of this plume and its tapering through a fine connecting filament to a larger blob of material.

The main difference between the two results are in the presence of another kink in the interface, that has developed just above the initial starting position at time t = 0.95 s. In the simulation of López *et al*³⁰ the interface drops smoothly downward from its position on the high left to the downward plume on the right side of the domain. These discrepancies are due to the different natures of both schemes and are probably dependent upon how compressive or diffusive the scheme is in its treatment of the interface.

7 CONCLUDING REMARKS

The scheme introduced in this report is based on the Compressive Interface Capturing scheme for Arbitrary Meshes (CICSAM) of Ubbink & Issa.²² The scheme switches smoothly between the upper bound of the universal limiter¹⁸ and ULTIMATE-QUICK, a combination

of the universal limiter and QUICK,²⁷ dependent upon the angle between the interface and the direction of motion.

Numerical results for four main test cases have been presented. In the first two cases, prescribed velocity fields were used and the current scheme outperformed six other methods tested by Rudman¹⁵ and Ubbink & Issa²² for comparison. In the final test cases, the advection equation for the volume fraction was coupled to the Navier-Stokes equations and two real fluid flow problems were examined. Test case three examined the collapse of liquid columns under gravity, representing various dam-breaks. It was found that simulation data for the position of the advancing water front and for the residual height of the column against time, accurately modelled that presented in an experimental investigation by Martin & Moyce.²⁹ Additionally, qualitative results for the nature of the flow during the dam-break indicated the presence of horizontal jets above the boundary, an effect observed in an experimental investigation by Stansby, Chegini & Barnes.¹ In the final test case, a Rayleigh-Taylor instability problem was investigated and the qualitative results obtained agreed with those observed in numerical simulations by López *et al.*³⁰

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