Numerical simulation of viscous free surface flow

S.E. Navti, R.W. Lewis and C. Taylor
Institute for Numerical Methods in Engineering, University of Wales, Swansea, UK

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1. Overview

Numerical modelling of mould filling during the casting of metals into moulds is a moving boundary problem, where the domain of interest has an unknown boundary at the start of the analysis. This type of problem has many important industrial applications. They include applications in capillarity, melting and solidification, crystal growth, flame propagation, nuclear fusion, wetting, seepage, glass and metal forming processes, and many others in engineering and science. An in-depth understanding of the physical phenomena which takes place at the free surface is necessary, if it is to be accurately modelled. Owing to the moving boundaries, and the complex physical processes at the free surface, difficulties are experienced when an attempt is made to track it, *viz*:

- A variety of interface conditions exist, e.g. oxide formation, surface tension etc., some of which might be non-linear.
- The solution domain is irregular, constantly changing and undergoing large distortions. This could typically result in break up of the fluid mass into droplets, or overlapping interfaces, resulting in the formation of air pockets.
- Surface tension effects have been found to depend on the curvature of the interface. As a result, in order to accurately predict the surface tension forces, the free surface has to be accurately modelled.
- The domain might contain internal obstacles or cores that need to be taken into account during free surface tracking.

Several approaches to free surface modelling have been attempted with varying degrees of success. These can be conveniently divided into two categories; the fixed and moving mesh types. The fixed mesh approaches are Eulerian and the moving mesh types Lagrangian. In the next two sections, the implementation of each of these methods will be described, along with a brief evaluation of the advantages and disadvantages.

1.1 Lagrangian method

This is the natural choice for moving boundary type problems (Donea, 1983; Hirt *et al.*, 1974; Ramaswamy and Kawahara, 1987). In this formulation, the coordinate system moves with the fluid. These methods are particularly suited to problems where the mesh does not experience significant distortion. The

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main attraction for the Lagrangian formulation is that it permits the material interface to be specifically delineated and precisely followed, and also allows interface boundary conditions to be precisely applied. Regions of high gradients can be refined, and allowed to move with the flow, resulting in an improvement in results. The Lagrangian formulation has been used by many authors for solving fluid flow problems (Hirt *et al.,* 1970; Schulz, 1964).

However, the main difficulty in dealing with the Lagrangian approach lies with mesh entanglement and numerical instability due to the irregular nature of the mesh. The first problem arises because a mesh of fixed topology quickly becomes distorted as the free surface deforms. This can be solved by re-meshing or rezoning, but doing so results in the re-emergence of the convective flux problem characteristics of the Eulerian approach. In addition, a robust re-meshing algorithm is essential for this method to be successful, ensuring that the variables are accurately transferred onto the finite element mesh for the next time step. Since general rezoning can be a very complex process, it is preferable to either use meshes that preserve the topology during the rezoning process, or to use continuous rezoning to take advantage of the simplifications offered by the small relative mesh displacements. Hirt *et al.* (1974) have implemented a continuous re-meshing algorithm using the finite volume technique. This approach, known as the Arbitrary Lagrangian-Eulerian method, in common with Eulerian methods, suffers from numerical diffusion. Margolin and Nichols have suggested ways of overcoming this problem. A similar front tracking model has been developed by Muttin *et al.* (1993). In summary, the Arbitrary Lagrangian-Eulerian formulation is a variant of the Lagrangian formulation, with the mesh deforming in terms of an arbitrary velocity, independent of the flow velocities, except at the free surface. The speed of the moving mesh is incorporated into the convective term, making it more stable numerically, and significantly reducing mesh distortions. The selection of the mesh velocity is, however, not trivial and requires an experienced user for proper implementation. The interface is tracked by following the Lagrangian motion of the vertices aligned initially with the interface. Displacements at the free surface have to be limited, and the method is more suitable for use with triangular elements. The good news is that there is no limit on the time step size and re-meshing can be restricted to either specified intervals or when significant mesh deformation has occurred. The Arbitrary Lagrangian-Eulerian formulation has been used by various authors for solving fluid flow problems (Bach and Hassinger, 1985; Brackbill and Saltzman, 1986; Hirt *et al.,* 1970; Hwang and Stöehr, 1988; Ramshaw, 1985).

The free surface has also been tracked along preselected splines. However, due to the complex nature of the filling patterns in mould filling, the above method would be difficult to implement, since the generation of appropriate splines requires some knowledge of the filling pattern (Debbaut, 1993; Kheshgi and Scriven, 1982). Discrete representations of viscous flow phenomena has been simulated using interacting particles. In this method, each particle has a set of attributes such as mass, position, velocity and momentum. The state of the fluid system is defined by the attributes of a finite assembly of particles and the evolution of the system defined by laws governing the interaction of particles. Since particles are associated with different material properties, the interface between materials can be easily followed. A review of this method can be found in reference (Floryan and Rasmussen, 1989).

All the moving mesh methods described above have additional requirements regarding the treatment of contact with the enclosing wall, and apart from the pure Lagrangian method, they all introduce truncation errors during the interpolation of variables from the distorted mesh to the new mesh.

1.2 Eulerian method

In the Eulerian formulation, the coordinate system is stationary, or moving in a certain prescribed manner in order to take into account the continuously changing solution domain. The grid movement is thus independent of the fluid particle movement. This results in the method being able to deal easily with fluids that undergo large distortions at the interface. Various variants of the Eulerian approach exist.

In the strictly Eulerian approach, the grid does not change. The method can thus cope with multiple interfaces and can handle large deformations without loss of accuracy. A main drawback of this method, however, lies in the fact that the interface location cannot be accurately determined since it does not lie on a grid line. Compared with the Lagrangian formulation, interface boundary conditions are more difficult to implement, although its treatment in 3D would be more straightforward. Hirt and Nichols (1981) have used the Eulerian approach to track the free surface. A method known as the surface tracking method is discussed in reference (Floryan and Rasmussen, 1989). In this method, the interface is represented by a series of interpolated curves through a discrete set of points. The method allows for the resolution of features of the interface smaller than the grid spacing. The main drawback of this method lies in the high memory requirements. At each time step, the location of the points, their connectivity, orientation and curvature has to be stored. This makes it very difficult to implement for highly deforming and intersecting free surfaces. As with the Lagrangian approach, the implementation of this method in three dimensions would be very difficult indeed. Other methods known as volume tracking methods are based on marker quantities which are used to indicate the state of the cells used to discretise the domain of interest. They have the advantage of not requiring storage of a representation of the interface. A method known as the MAC method has also been developed (Harlow and Welch, 1965; Welch *et al.,* 1965). In this method, massless marker particles are used to identify the free surface. Cells containing these marker particles are known to lie on the interface. The main drawback of this method lies in the fact that the resolution of the interface is limited to the mesh size, and in addition, no information is available on the orientation and curvature of the free surface. As well as maintaining a grid, additional marker particles are necessary, which makes the method computationally expensive. Another disadvantage lies in the fact that interface boundary conditions are difficult to implement. However, the method can treat any number of fluids and can also simulate interacting surfaces undergoing large distortions. A fraction volume of a cell occupied by one of the fluids can also be used as a marker particle. The main difficulty with this is that, since only one piece of information is available regarding the interface per cell, a certain arbitrariness in reconstructing the shape of the interface has to be allowed. This no doubt, introduces errors, the extent of which is difficult to judge (Barr and Ashurst). Noh and Woodward developed the simple line interface calculation (SLIC) algorithm in which the cells are partitioned by straight lines according to some fractional volume. The fluid velocities are used to increment the interface in the normal direction. Various authors have used the SLIC algorithm to varying degrees (Chorin, 1980; 1985; Sethian, 1985; Youngs, 1975). Another variant of this approach is the volume of fluid (VOF) method by Hirt and Nichols (1981). In this approach, a function $F(x, y;t)$ is defined such that an iso-value contour indicates the interface location. The discontinuity in F across the interface is propagated using the expression,

$$\frac{\partial F}{\partial t} + \mathbf{u}.(\nabla F) = 0 \tag{1}$$

This algorithm is similar to the SLIC method in that the interface is approximated by a contour, passing through the interface surface elements. As with the methods just discussed, the VOF method does not resolve details of the interface that are smaller than the mesh size. In addition, the curvature of the interface cannot be accurately determined. The slope of the interface is determined by the average value of F in the interface elements. The main plus for this method lies in its robustness and ability to treat multiple interfaces. Temporary holes and a Darcy type law has been used to allow air to filter through the porous mould walls as is the case for sand castings. In both cases, an experienced user is needed for the resulting filling pattern to be realistic. The grid can be adjusted adaptively in some cases to coincide locally with the interface. This would no doubt, result in a higher resolution of the interface. Information on the orientation and local curvature of the curves defining the interface would then be readily available. The interface can then be tracked by moving the interface mesh points in a Lagrangian manner. This method would also allow for adaptivity in the interior of the solution domain, significantly improving accuracy and resolution. The method used to adjust the mesh points at the interface is, however, not trivial and would be difficult to implement for highly deformed interfaces. A form of mapping could also be used, in which the independent variable is used to transform the irregularly shaped domain into a regularly shaped computational domain before discretisation of the governing equations. The mapping function thus occurs explicitly as one of the unknown functions in the system of governing equations. The problem is thus a fixed domain problem, and maintains a sharp resolution at the interface, but its application would be limited to geometries that do not result in singular mappings. A review of the implementation of mapping algorithms can be found in reference (Floryan and Rasmussen, 1989). Another free surface tracking method in this category is named fringe element generation. Here, fringe elements are generated temporarily at the free surface so boundary conditions are more accurately satisfied. A net inflow method has been applied to simulate time dependent free surface flows (Wang and Wang, 1994). In this method, both filled and unfilled domains are included in the analysis, with the volume of the incompressible liquid in each control volume calculated at each iteration. Finite element formulations have also been developed for simulating metal casting flows using the fixed mesh approach (Backer, 1993; Broyer *et al.,* 1995; Codina *et al.,* 1994; Gao *et al.,* 1989; Hartin, 1993; Kreziak *et al.,* 1993; Lin and Tsai, 1993; Lipinski *et al.,* 1993; Minaie *et al.,* 1987; Ohnaka, 1993; Swaminathan and Voller, 1993; Tadayon *et al.,* 1993; Usmani *et al.,* 1992; Waite and Sammonds, 1993; Zhang and Liu, 1993). As with the Lagrangian formulation, the method of choice depends on the type of problem being modelled.

2. Physical model

The equations governing the problem to be solved are the incompressibility condition

$$\nabla.\mathbf{u} = 0 \tag{2}$$

and the transport of fluid momentum, *viz;*

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}.\nabla)\mathbf{u}\right) - \tau + \nabla p = \mathbf{f} \tag{3}$$

where **u** denotes the fluid velocity, ρ the density, p the scalar pressure, **f** the body force (ρg) and τ the viscous stress tensor.

Boundary conditions are applicable to the Navier Stokes equations as specified velocities or pressure at the boundaries. These may be constant or allowed to vary with time. In the problems described, pressure is specified as atmospheric on the outlet boundaries, or free surface. At the neighbourhood of the contact line, where the fluid interface intersects the solid boundaries, conventional fluid mechanics indicates that the stress would become infinite (Huh and Scriven, 1971). In all the examples dealt with in this work, slip boundary conditions are used. This is due to the assumption that the boundary layer has little effect on the flow pattern for mould filling problems. In addition, modelling the fluid flow within the boundary layer requires a large number of elements, significantly increasing the solution CPU time. The singularity at the contact line is thus avoided when this class of boundary condition is used.

3. Numerical model

The conventional Galerkin weighted residual technique is used to obtain a discretised form of the governing equations. These were then approximated using the mixed interpolation formulation so that variables could be reduced by elimination. Details on the numerical model implemented can be found in references (Lewis *et al.,* 1997; Navti, 1996; Navti *et al.,* 1997).

4. Lagrangian front tracking algorithm

The updated free surface Lagrangian-Eulerian finite element kinematic description is used to modelling free surface flow in geometries where free surface boundary conditions are important. The model is based on an Eulerian finite element formulation applied to the solution of the Navier Stokes equations, combined with a Lagrangian free surface incrementation/tracking method. The principal advantage of this method lies in the natural representation of the free surface. The points defining the boundary are not tied together for the duration of the calculation, but can be deleted, added or reconnected as desired. The efficiency of the mesh generator is crucial in ensuring that the time saved in ommiting computations in the air domain are not used up in re-meshing the domain. In order to be free from topological constraints, the mesh employed in two dimensions, is, essentially triangular. The CPU time required for mesh generation is small when compared with the solution time. In fact, in most cases, significant saving in CPU time can be obtained over other fixed mesh approaches by virtue of the air domain being ignored. For most practical examples, the meshing accounts for approximately 15 per cent cpu time, while 80 per cent is spent in the solution phase. A full description of the method, along with the approach used to automatically assign boundary conditions to the changing domain is described in references (Lewis *et al.,* 1997; Navti, 1996; Navti *et al.,* 1997).

5. Numerical examples

5.1 Analysis of a solitary wave propagation

The analysis of the propagation of a solitary wave, used by Ramaswamy and Kawahara (1987) to validate his model, is presented in this section. The reader is advised to refer to Ramaswamy's paper for references on the solitary wave propagation problem, and a description of Laitone’s approximation, commonly used for comparative study. It allows testing of the ability of the Lagrangian free surface tracking algorithm and the finite element formulation in modelling free surface flow problems with respect to time and displacement.

The dimensions of the problem analysed in this study is shown in Figure 1. The time step used for the analysis was 0.050s, viscosity 1.0kg/ms, and density 1.0kg/m^3. A gravitational acceleration of magnitude 9.8m/s^2 acts in the vertical downward direction. The aim of the study was to compare the run-up height, R, of a solitary wave on a vertical wall. For the chosen dimensions, the initial conditions at t = 0 secs can be obtained from Laitone’s approximation. These can be written as

$$
\begin{aligned}
u &= 1.979898987\,(sech^2\,(0.03872983346x))\\
v &= 0.1533623161y(sech^2(0.03872983346x))tanh(0.03872983346x)\\
\eta &= 10.0 + 2.0sech^2(0.03872983346x)\\
p &= 9.8((10.0 + 2.0sech^2(0.03872983346x)) - y)
\end{aligned}
\tag{4}
$$

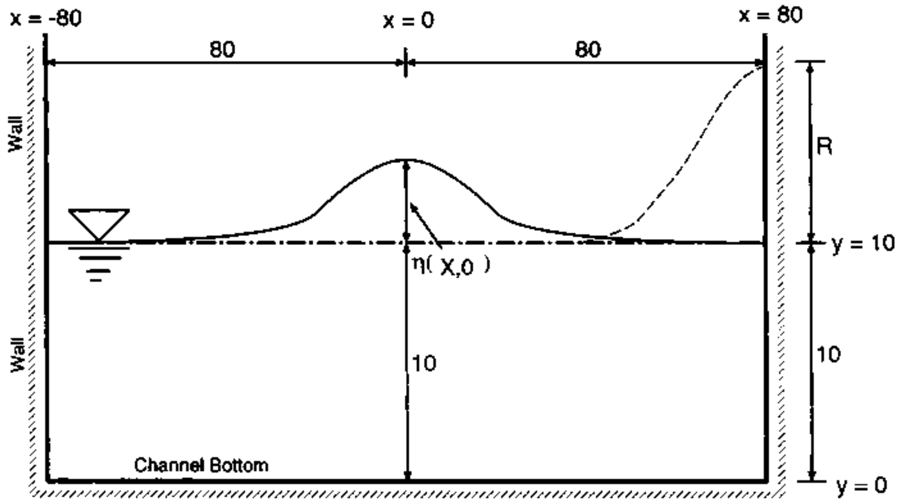

Figure 1.
Problem definition for solitary wave propagation

where x and y are the coordinates of the mesh points, u and v the local point velocities in the x and y cartesian coordinate directions, η the free surface elevation, and p the pressure. The general form of the approximations can be found in reference (Ramaswamy and Kawahara, 1987).

The initial condition is shown in Figure 2, where the wave is moving horizontally under hydrostatic pressure. The features observed at subsequent time steps are presented in Figures 3 and 4. Figure 4 indicates that the wave hits the right wall between t = 6.0s and t = 8.0s. A more accurate value can be obtained by referring to Figure 5, i.e. t = 7.6s, when the rise-up height begins to drop. A value of t = 7.7s was predicted by Ramaswamy and Kamahara (1987). The rise-up at the point of impact was computed as R = 3.4, see Figure 5, compared with R = 4.2 obtained using Laitone's approximation. A subsequent analysis using a viscosity of 10.0kg/ms predicted a rise-up height of R = 3.12. This confirms that the viscous effects of the fluid modelled have an effect on the rise-up height at the wall, and is attributed to be the reason why the rise-up height does not compare directly with the results presented by Ramaswamy and Kawahara (1987). Further computations at a viscosity of 0.1kg/ms were attempted, but did not converge for the current mesh prescription.

5.2 Filling of an axisymmetric wheel casting

The geometry of the axisymmetric pulley wheel problem is shown in Figure 6. The material properties used were that of Al, density 2560kg/m^3 and viscosity 1.7kg m^{-1}s. In order to simulate the clearly turbulent nature of the flow using the proposed laminar flow algorithm, a fictitious dynamic viscosity, 1,000 times the real viscosity has been used. The filling was performed against a gravitational force of 9.81m/s^2, and under the driving force of a specified inlet velocity of 0.31m/s. Slip boundary conditions were employed. The tolerance and

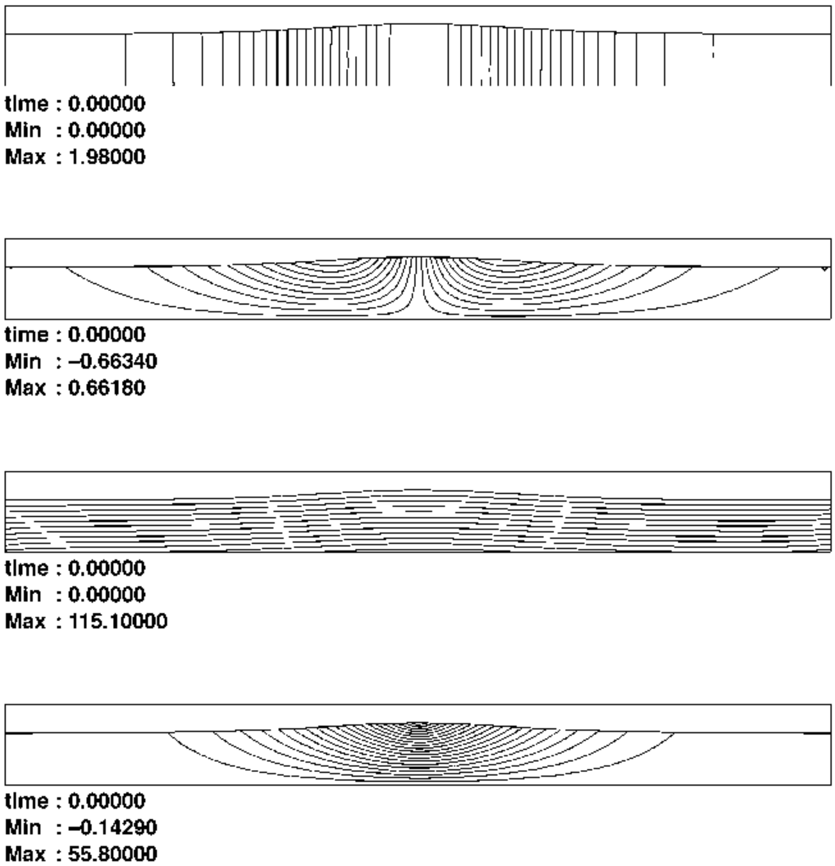

Figure 2.
Initial condition. From top to bottom; U velocity component distribution (m/s), V velocity component distribution (m/s), pressure (Pa) and streamline contour plots

relaxation parameters were set to 5 per cent and 0.5 respectively, with the mesh generated at every time step. The time step was automatically chosen in order to ensure that about 0.5 per cent of the mould cavity gets filled at each time step. The selection of a constant maximum or minimum time step for the analysis as with the previous example, proved to be inadequate as the metal filled the domain. This was as a result of the much reduced free surface velocities, due to flow in the third dimension being modelled. The time step selection, as well as the mesh density were, therefore, automated, with the mesh density based on the amount of metal in the mould; the only limitation being that the number of elements must not exceed 2,000. This enables the program to be compiled without options required for checking array dimensions, resulting in a more efficient executable code. Throughout the analysis, the fluid loss due to wall penetration is continually monitored, and limited to 5.0 per cent of the fluid flowing in to the mould cavity.

Figures 7 to 10 show the results obtained for analysis. It can be noted that the free surface has a fairly flat profile. The filling is at a constant rate for all

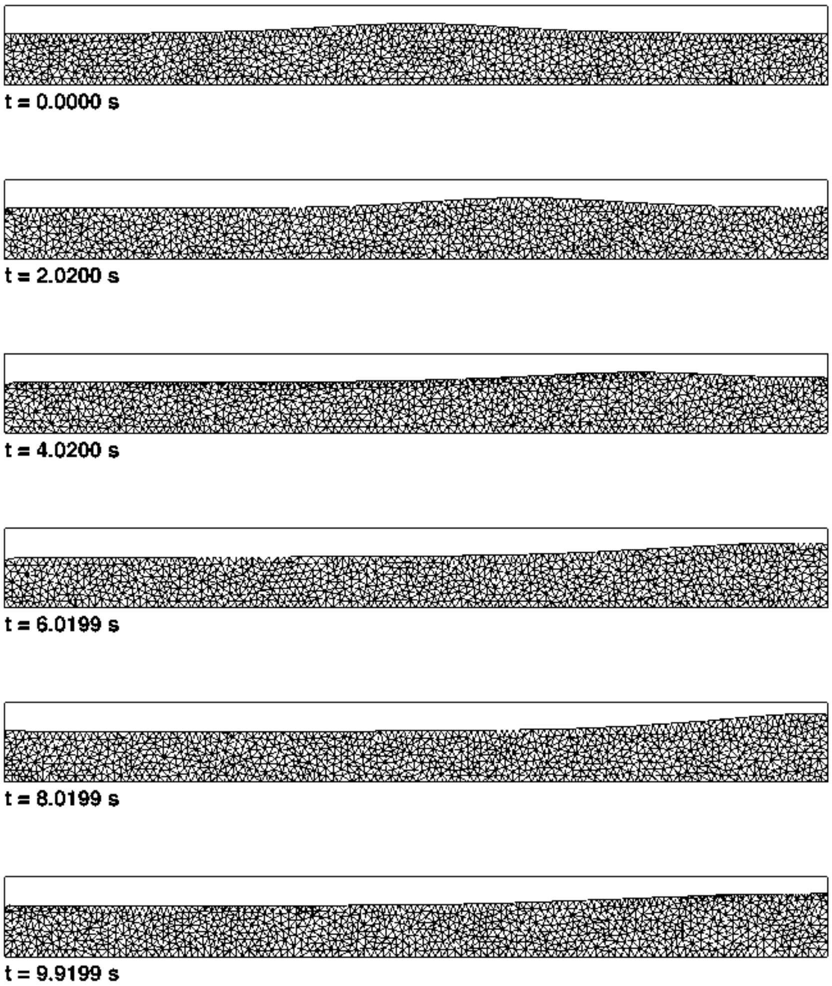

Figure 3.
Mesh/front plots

sections of the casting for this analysis. The axisymmetric nature of the casting results in low velocities in the interior of the mould cavity, when compared to the velocity in the ingate. Some re-circulatory flow patterns are observed in the analysis, evident from the stream line contour plots. The dominant effect of gravity can be appreciated from the pressure contour plot.

5.3 Filling of a simple gravity tilt-pour casting

In this section, the filling of a plate casting, containing an internal core is analysed. Filling is initiated by tilting the mould cavity. This enables the pourer to adjust the tilting speed so as to avoid surface turbulence and air entrapment. Here, the pouring cup is initially filled with molten tin, at 400°C. Tilting the

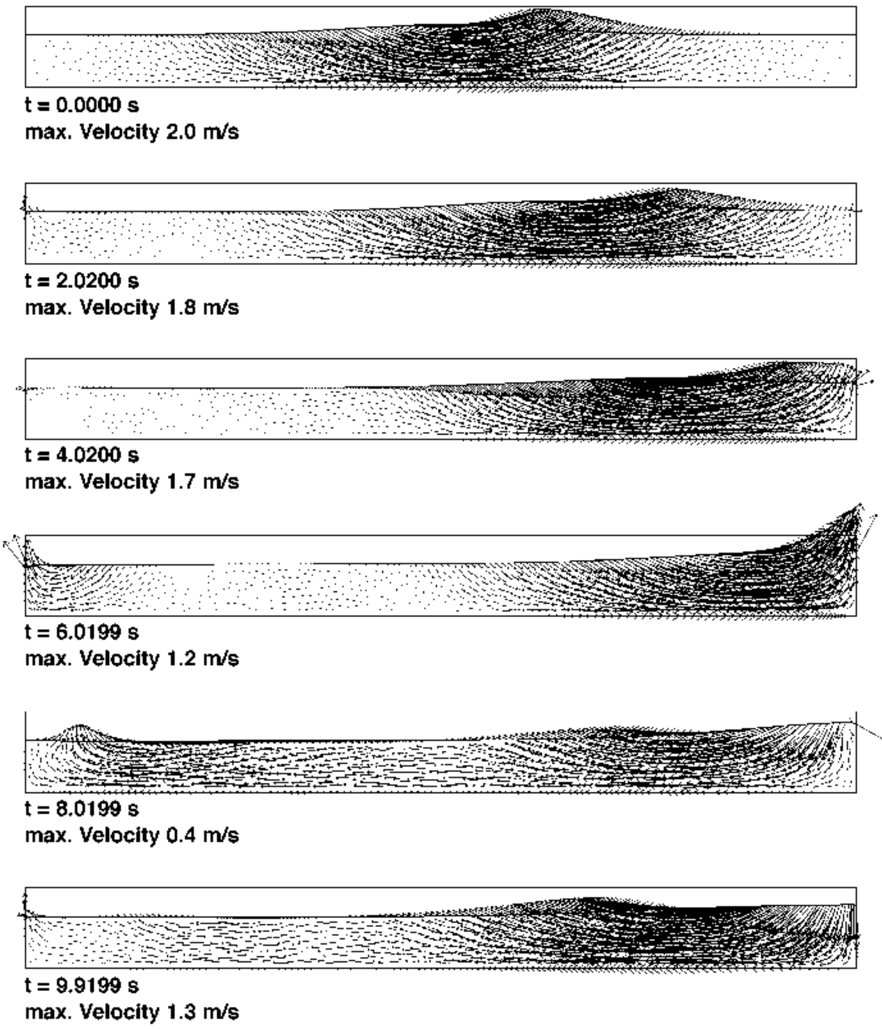

Figure 4.
Velocity vector plots

experimental setup about its centre of gravity results in a controlled filling of the mould cavity. Numerical results obtained can be compared to experimentally derived filling results (Kim and Hong, 1995). The geometry of the casting and setup is shown in Figure 11. In the experimental setup (see Kim and Hong, 1995), the mechanical drive for the tilting system was provided by variable speed electric motor. As in the experiment, the whole mould assembly is rotated through a set angle, starting from a horizontal to a vertical position, i.e. 0-90° rotation. The dimensions of the plate casting was $200 \times 100 \times 10$mm. The material properties used were, density 6840kg/m^3 and viscosity 1.97kgm^{-1}s. The driving force of the flow was gravity, 9.81m/s^2, acting in the

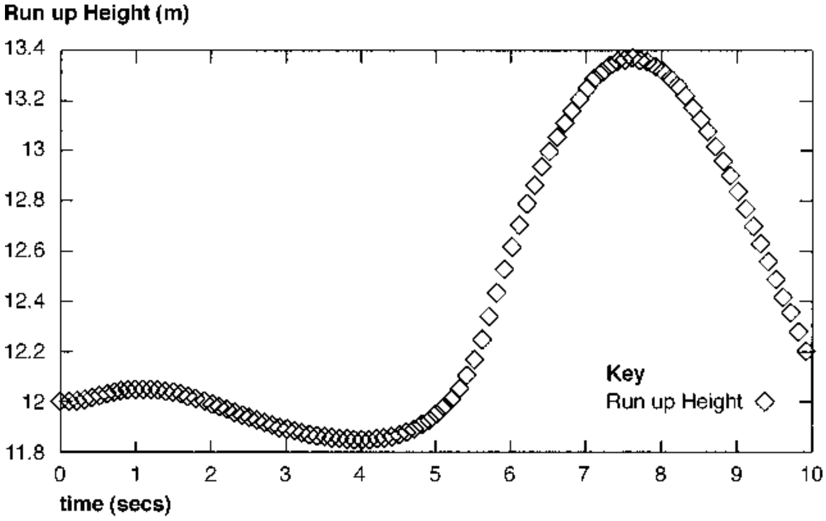

Figure 5.
Run-up height

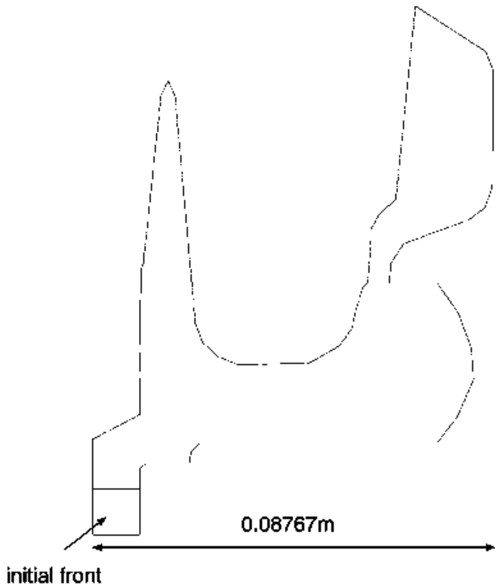

Figure 6.
Casting geometry and initial front

vertical downward direction. Slip boundary conditions were employed. The tolerance and relaxation parameters used were identical to those in the previous example, with the mesh generated at every time step. The time step was allowed to vary between 0.001 and 0.005*s*, depending on the distance of the closest free surface node to the wall, and the allowable fluid loss due to penetration, currently 5 per cent of the instantaneous volume of fluid flowing into the mould cavity.

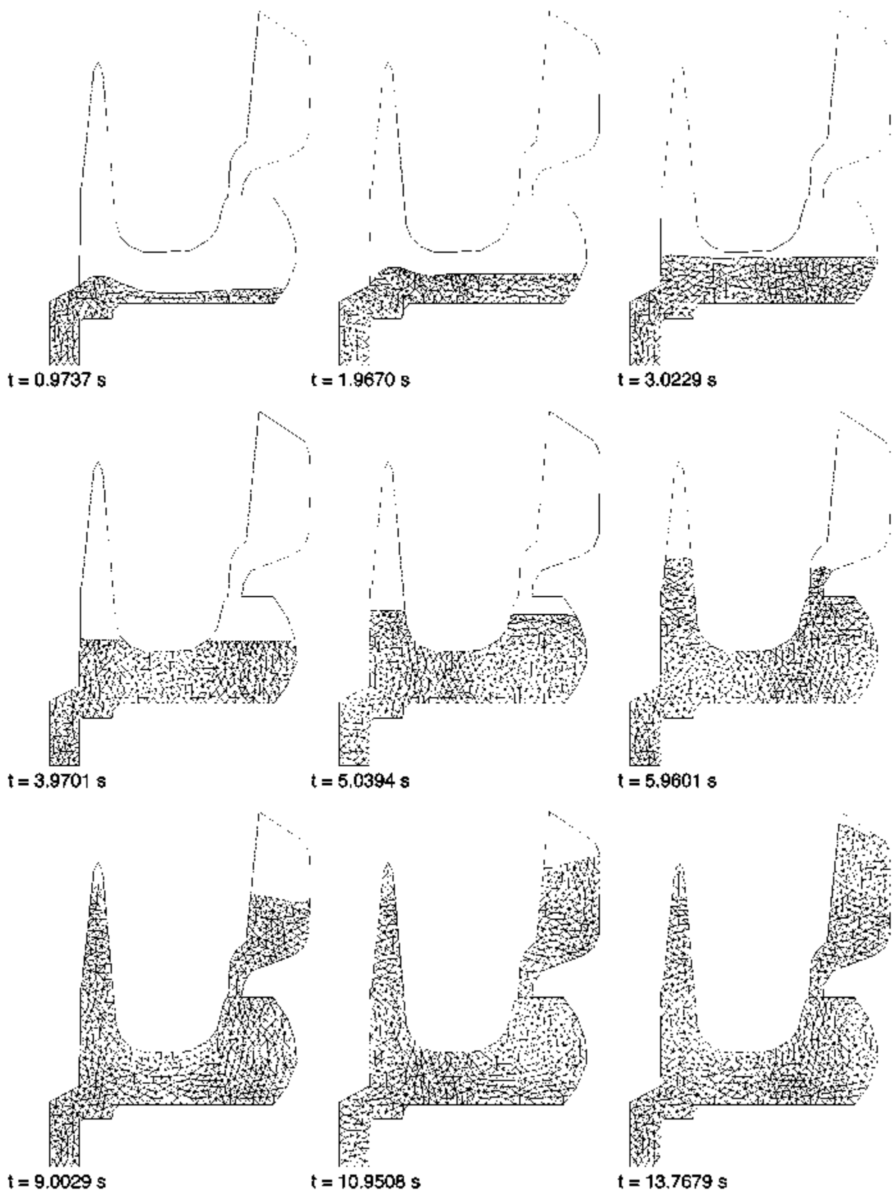

Figure 7.
Mesh plots for 3-D analysis

Results obtained from the numerical analysis are shown in Figures 12 to 13. Although the results presented by Kim and Hong are insufficient for a conclusive validation of the tilt pouring algorithm, the free surface profile at the selected time steps are similar to those obtained during the experiment. Tilting results in a uniform filling rate, with the maximum free surface velocity maintained at below 1.0m/s, ideal for mould filling.

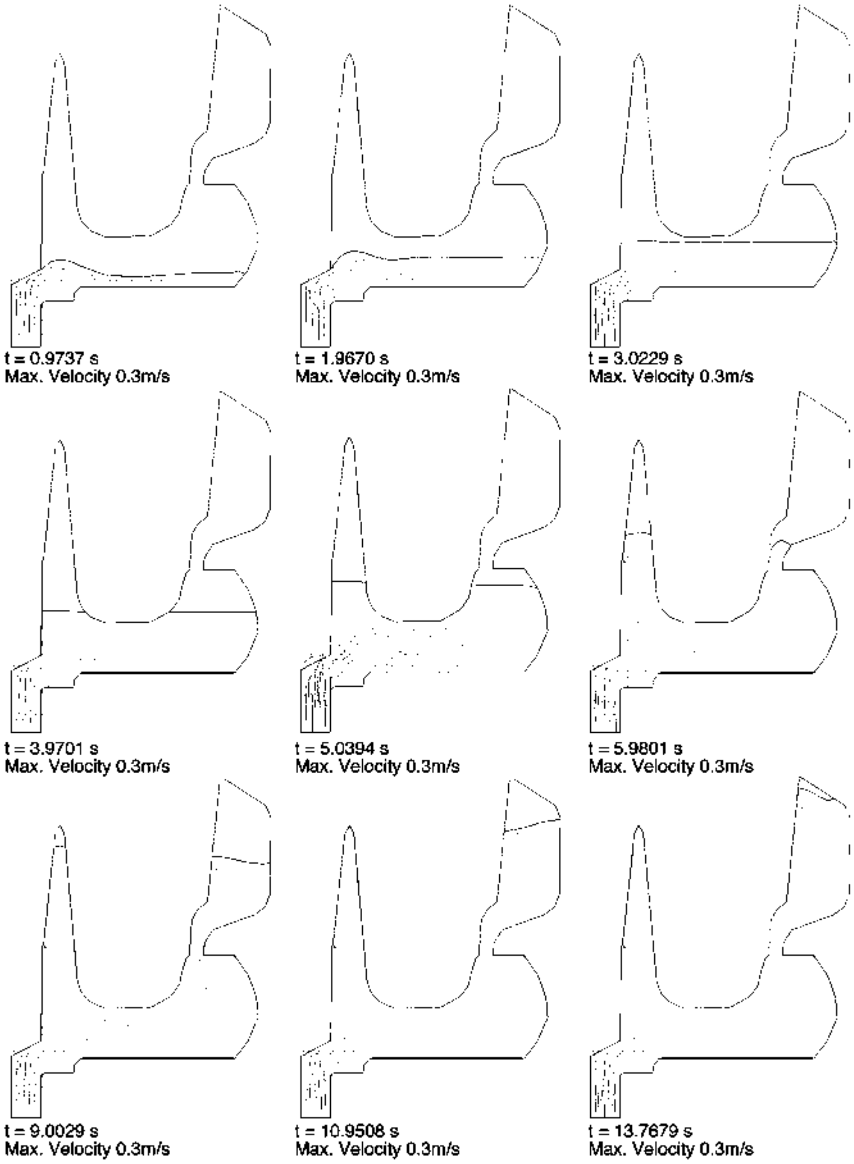

Figure 8.
Velocity vector plots for 3-D analysis

6. Conclusion

The effectiveness of an updated free surface Lagrangian-Eulerian finite element kinematic description in simulating free surface flow problems, particularly mould filling, has been demonstrated. A mixed interpolation formulation has been successfully used to approximate the discretised the governing equations for elimination, on a Lagrangian type moving mesh. Significant savings in CPU

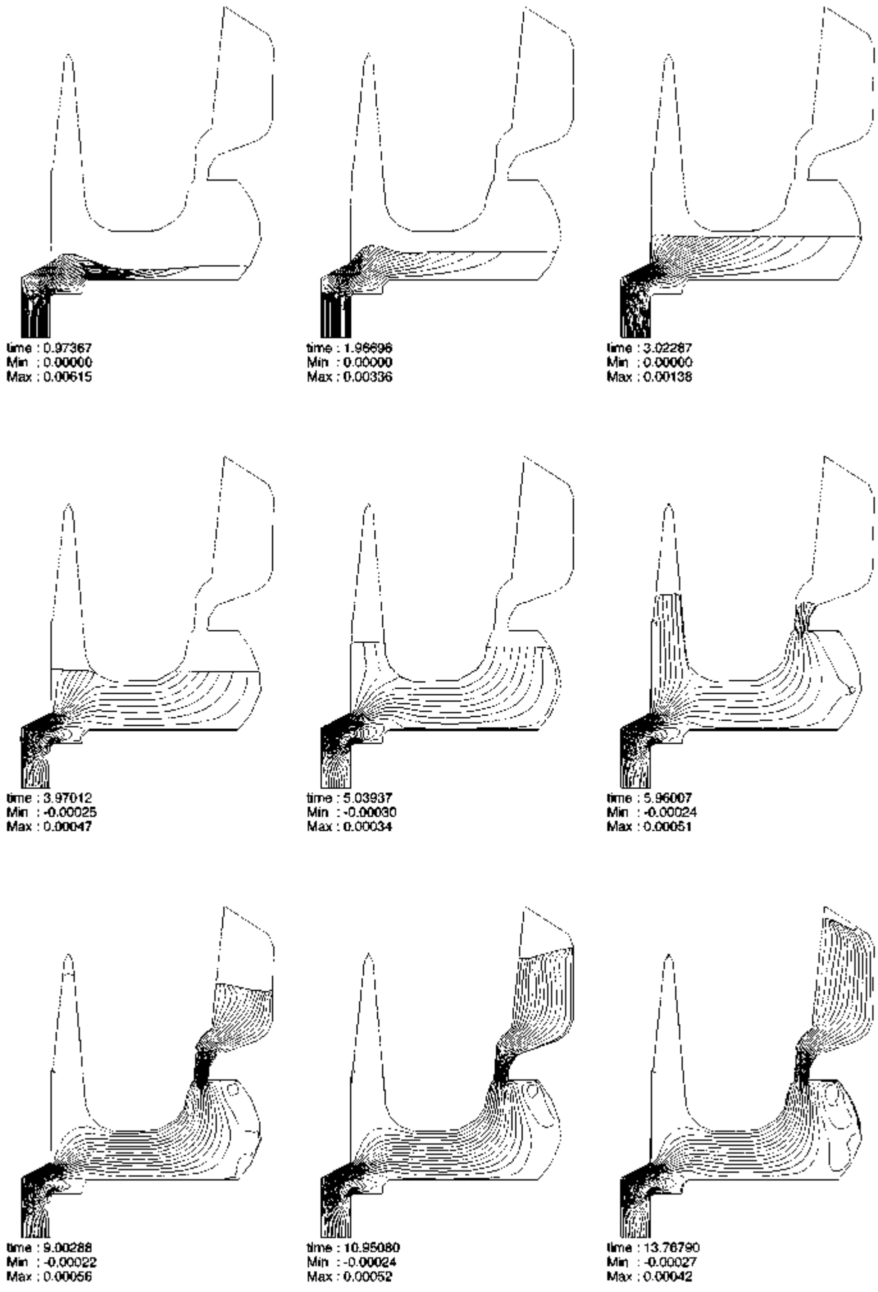

Figure 9.
Stream line contour plots for 3-D analysis (time in secs)

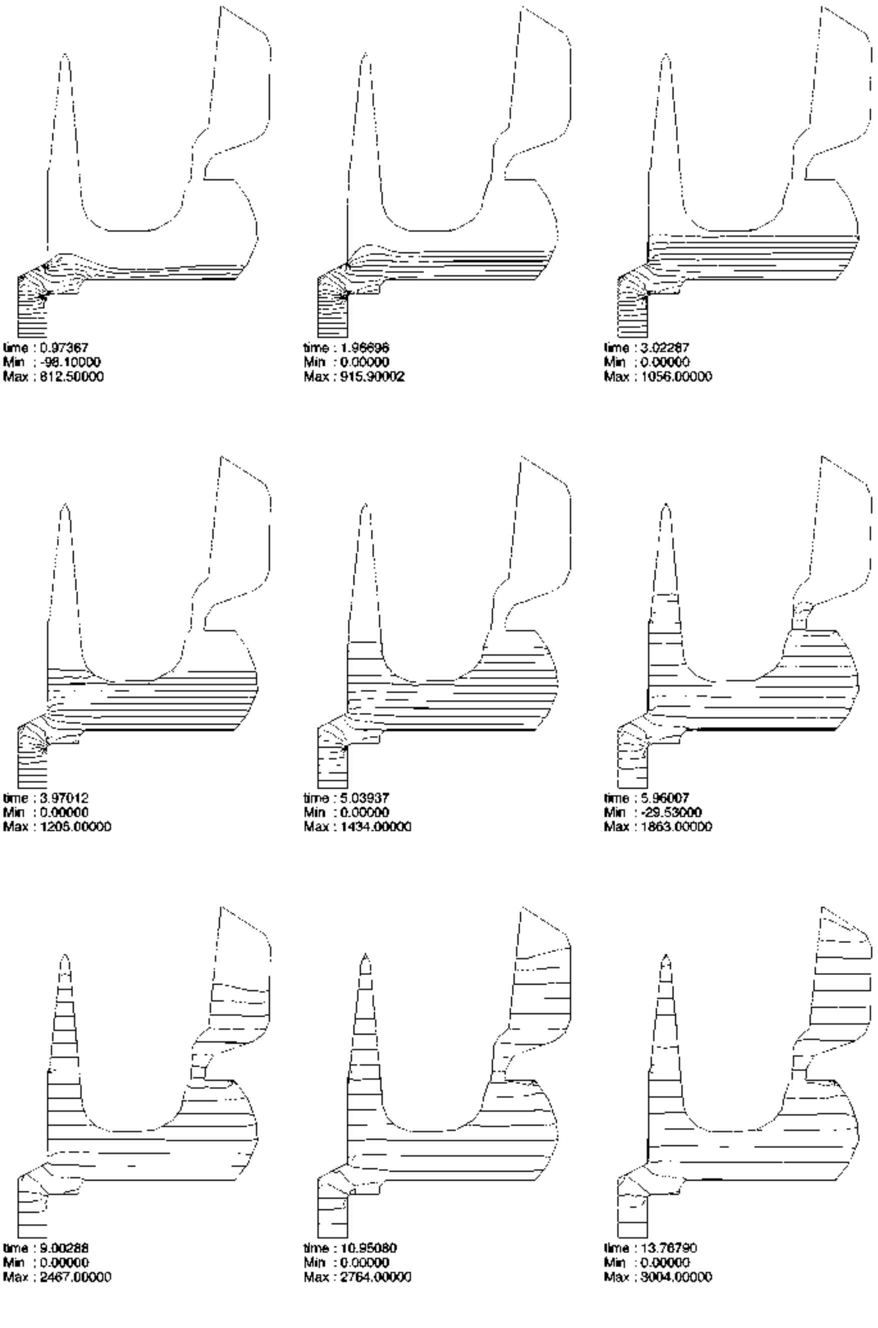

Figure 10.
Pressure contour plots (Pa) for 3-D analysis (time in secs)

time are realised, by virtue of the air domain not being considered in the finite element analysis; unlike with the VOF method, an explicit determination of the free surface results, making it ideal for the application of free surface boundary

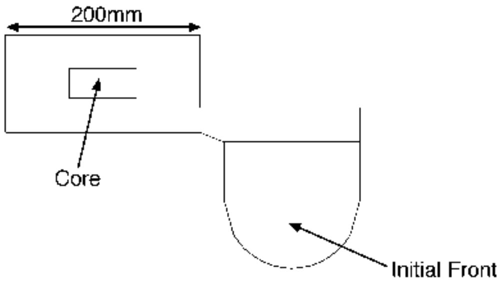

Figure 11.
Mould setup and initial front

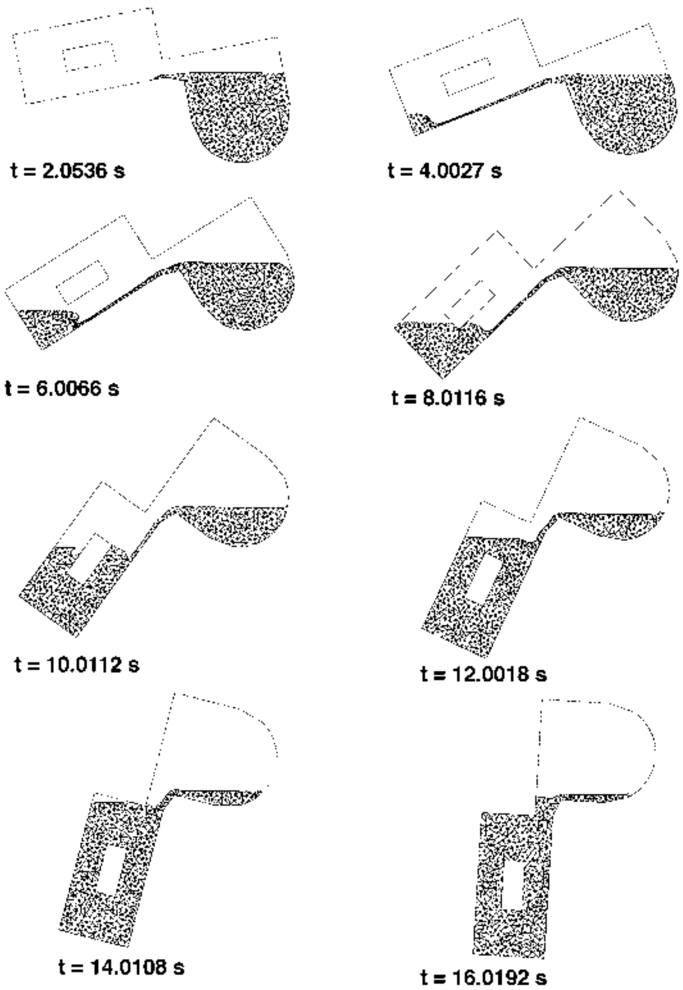

Figure 12.
Mesh plots for tilt-pour analysis

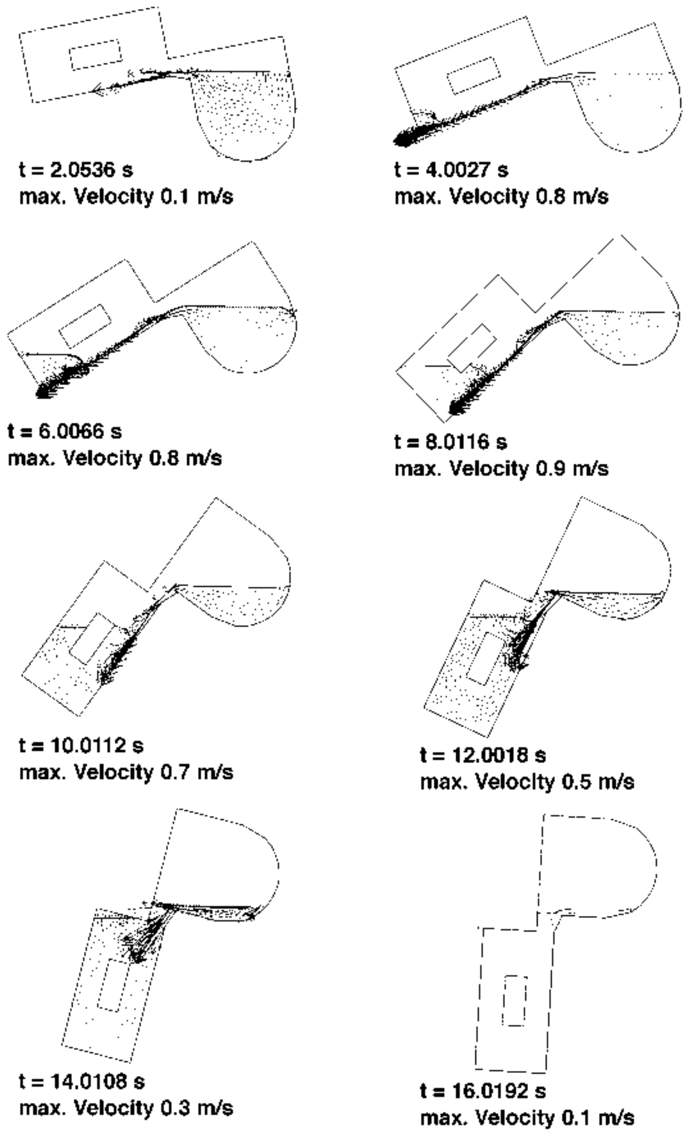

Figure 13.
Velocity vector plots for tilt-pour analysis

conditions. Difficulties associated with tracking the free surface would be significantly reduced if the above method is applied to the modelling of engineering processes where the free surface experiences less distortion.

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