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AN ADVECTION SCHEME FOR USING THE LAGRANGIAN REMAP IN VOLUME TRACKING METHODS ON ARBITRARY MESHES

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Abstract. In this paper, an advection scheme for using the Lagrangian remap is proposed. This proposed scheme can be used on arbitrary meshes composed of any polyhedron. The formulation of the scheme is described and results of numerical tests carried out are shown. The results of those numerical tests revealed that the proposed scheme can evaluate transported volumes without any procedures out of its formulation. Finally, a turbulent flow with free-surface in a stirred vessel with baffles was analysed. In this analysis, ALE method and a mesh with discontinuous boundaries were used. The proposed scheme for volume tracking can be used cooperating with those method and mesh without losing of the accuracy.

Key words: Advection, Lagrangian remap, VOF, Volume tracking, Unstructured meshes

1. INTRODUCTION

VOF (Volume of fluid) method has widely been used for analysing free-surface flows. Although different schemes for discritising the advection equation used in VOF method have also been proposed, most of them are for analysing on structured meshes. They are based on fluxing schemes, which evaluate transported volumes through cell boundaries. If a similar scheme is applied on unstructured meshes, the resultant scheme would be complex one; Accordingly, CICSAM (Compressible Interface Capturing Scheme on Arbitrary Meshes) scheme [1], which can be used on unstructured meshes, is not based on volume tracking but based on a high resolution method.

On the other hand, methods using the Lagrangian remap [2] can evaluate transported volumes in volume tracking frameworks. However, if volumes of a fluid are tracked in some formulations using the Lagrangian remap, intolerable errors are caused because of local volume defect. As a result, we need some procedures to correct the errors out of formulation used. The purpose of this paper is to provide a general and accurate scheme for using the Lagrangian remap regardless of whether analysing on structured or unstructured meshes. The proposed scheme is closed in its formulation and does not need any procedures to correct the error induced by incomplete formulation in the discritised advection equation.

This paper consists of the following sections. The proposed advection scheme is described in detail in the section 2. In the section 3, numerical tests are carried out and the calculation results are compared with analytical and experimental results. In the section 4, the proposed scheme is used to analyse a turbulent flow with free-surface in a stirred vessel with baffles. In this analysis, ALE (Arbitrary Lagrangian-Eulerian) method is cooperated with the proposed scheme and a mesh with discontinuous boundaries is used. Conclusions obtained in this paper are described in the last section.

2. THE ADVECTION SHCEME

2.1 The volume tracking frameworks

The equation described free-surface flows in VOF (Volume of Fluid) method is the following advection equation.

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial x_i} = 0 . \tag{1}$$

F stands for volume fraction of a fluid in a cell and fluids are represented by value of F. If F is equal to 0 or 1, the fluid in that cell is fluid 1 or fluid 2 depending on the value of F. Thus interfaces exist in cells where F is greater than 0 and less than 1. This equation is integrated with respect to a cell Ω and a time interval with the continuity of incompressible fluid;

$$\int_{\Omega} \left(F^{n+1} - F^{n}\right) d\Omega + \int_{n}^{n+1} \int_{\Gamma} u_i F^{n} n_i d\Gamma dt = 0 , \tag{2}$$

where n_i is the outward normal vector of surface Γ of a cell and superscript n stands for time level. Equation (2) is discritised as follows:

$$F^{n+1} = F^{n} + \frac{\sum_{\Gamma} \delta F_{\Gamma}}{\delta V_{\Omega}} , \tag{3}$$

where $\delta F_{\Gamma} = u_i n_i \Delta\Gamma \Delta t$ is the transported volume through surface Γ of a cell and δV_{Ω} volume of a cell Ω. Generally, this equation is the discritised equation of the advection equation (1) on structured meshes. In order to evaluate the transported volumes through cell boundaries, the reconstruction of the interface is required. In PLIC (Piecewise Linear Interface Calculation) [3], the interface is approximated by a planar face and reconstructed in a cell instead of reconstructing at cell boundaries in mesh used.

The discritised equation (3) can be calculated in each spatial coordinate separately, which is referred to as operator-splitting methods. In the operator-splitting method used in [3], the divergence term is added in the advection equation (1):

$$\frac{\partial F}{\partial t} + \frac{\partial u_i F}{\partial x_i} = F \frac{\partial u_i}{\partial x_i} . \tag{4}$$

Note that the above equation (4) is discritised and calculated in each spatial coordinate separately and the calculation order of spatial coordinate is not important. The operator-splitting methods are no longer applicable on unstructured meshes, since each spatial dimension of mesh used does not necessarily correspond with spatial coordinates.

2.2 The advection scheme by means of the Lagrangian remap

In volume tracking frameworks, the transported volumes need to be evaluated in order to calculate the discritised advection equation. The transported volumes can be evaluated by

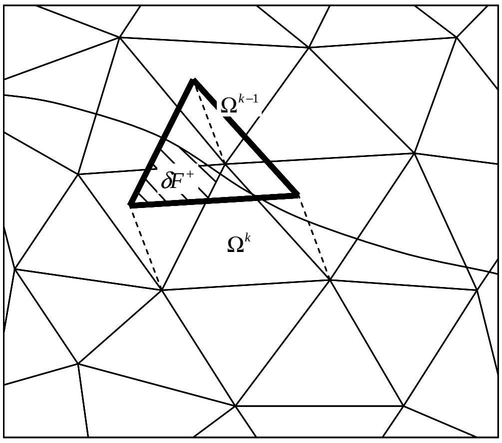


Fig. 1 *The Lagrangian remap. The cell* Ω *is moved along streamlines shown by dash-lines. Shaded area/volume is the transported volume of a fluid into the cell.*

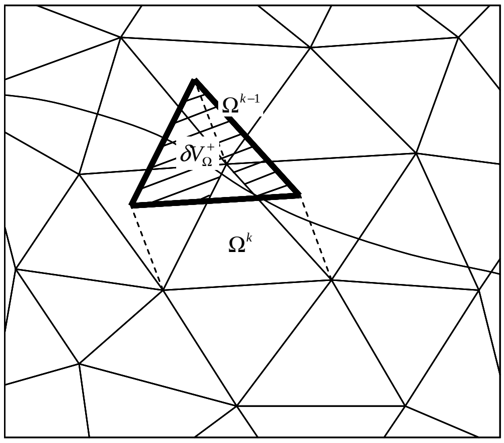


Fig. 2 *The geometric volume used in the proposed scheme. Shaded area/volume is evaluated for the geometric divergence term.*

means of the Lagrangian remap, while the transported volumes through cell boundaries are evaluated in flux-based schemes, as shown in Figure 1.

In the Lagrangian remap, vertices of a cell are moved along streamlines, which are shown by dash-lines in Figure 1. These streamlines are not necessarily straight lines even if the velocity field satisfies the continuity of incompressible flows, whereas so exactly in the case of that flows are translations.

The spatial coordinate x_i of a cell Ω is moved by using the following equation.

$$x_i^{k-1} = -\int_{k-1}^{k} u_i^k \, dt + x_i^k \,, \tag{5}$$

where superscript k stands for pseudo-time. Every cell is track backed by the 4th-order Runge-Kutta method. Therefore volume transported into a cell results in the volume of a fluid occupied in the Lagrangian prototype Ω^{k-1} overlapped into neighbour cells.

The advection equation discritised by means of the Lagrangian remap is similar one to the flux-based equation (3).

$$F^{n+1} = F^n + \frac{\delta F^+ - \delta F^-}{\delta V_\Omega} \,, \tag{6}$$

where δF^+ stands for inflow volume of a fluid into a cell and δF^- outflow volume of a fluid from a cell. The advection scheme (6) is essential to be followed a procedure called the repair algorithm to correct errors out of its formulation [2]. Because it is unable to reach solutions unless this repair step is involved. As the repair algorithm is used for preventing the error, however, the repair algorithm can lead to losing of the accuracy as well. This problem can be resolved by the following formulation used in the proposed scheme without repair algorithms.

The error caused by the equation (6), which leads to incorrect volume fractions, originates from the difference of volumes of the Lagrangian prototypes related to a cell Ω. Therefore a term is necessary for cancelling the error.

$$F^{n+1} = F^n + \frac{\delta F^+ - \delta F^-}{\delta V_\Omega} + D^n . \tag{7}$$

D is as follows:

$$D^n = F^n \frac{\delta V_\Omega^- - \delta V_\Omega^+}{\delta V_\Omega} , \tag{8}$$

where δV_Ω^+ stands for the volume of the Lagrangian prototype of the cell Ω which is overlapped into neighbour cells and δV_Ω^- the volume of the Lagrangian prototype of neighbour cells which is overlapped into the cell Ω, as shown in Figure 2. This formulation corresponds to the advection equation (4) used by the operator-splitting method on structured meshes. The difference between the operator-splitting method and the proposed advection scheme is how to evaluate the divergence term.

In the operator-splitting method used on structured meshes, the advection equation (4) is calculated in each spatial coordinate separately. Thus the sum of the right-hand side of the equation (4) is not zero. This procedure can not be applied to the equation (7) using the Lagrangian remap, since the divergence of velocity is zero due to the continuity of incompressible fluids. However D evaluated by the equation (8) has some values and plays the role of the right-hand side of the advection equation (4) separated in each spatial coordinate. Hence we call it the geometric divergence term.

Overestimation and underestimation of the transported volume are cancelled out because of this geometric divergence term. It is important that the proposed scheme is completed in its formulation and it does not need any procedures to correct inherent errors in schemes. In addition, the proposed scheme is applicable on arbitrary meshes composed of any polyhedron.

This scheme is stable and robust if the Courant number is only equal to or less than 1. Moreover, this scheme can be used even on meshes with discontinuous boundaries without any difficulties since it does not require any modifications for evaluating the transported volumes and the geometric divergence term (8), whereas this may not be the case if a flux-based scheme is used. The result using a mesh with discontinuous boundaries will be shown in the section 4.

3. NUMERICAL TESTS

In this section, numerical tests are carried out on meshes composed of hybrid cells in order to reveal the capability of the proposed scheme. Numerical tests carried out in this section are translation, rigid-body rotation and the broken-dam problem.

In translation and rigid-body rotation tests, the accuracy of the scheme is evaluated by the error norm E defined as follows:

$$E = \frac{\sum_\Omega \left\| F_\Omega^{calc} \delta V_\Omega - F_\Omega^{exact} \delta V_\Omega \right\|}{\sum_\Omega F_\Omega^{exact} \delta V_\Omega} , \tag{9}$$

where F_Ω^{calc} and F_Ω^{exact} are the calculated volume fraction and the exact one, respectively. In the broken-dam problem, the calculation result is compared with the experimental one. All tests were calculated in parallel.

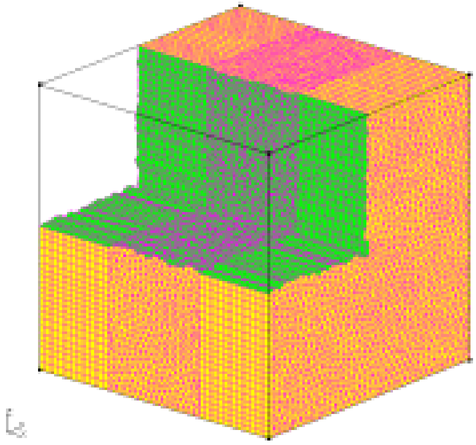


Fig. 3 *Mesh used in the translation tests. Typical element size of mesh shown is 0.02L.*

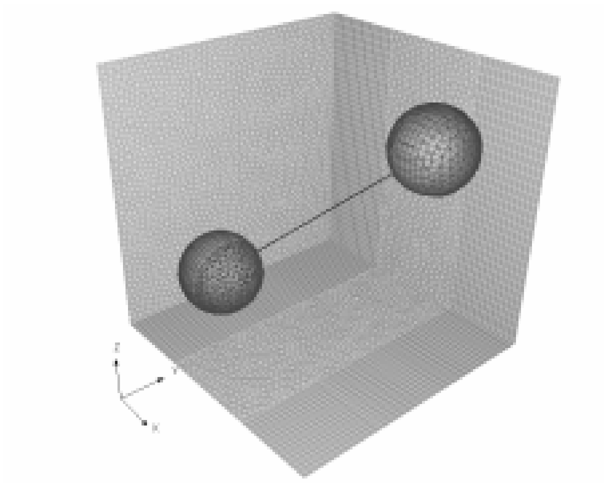


Fig. 4 *The result of the translation test. The sphere is moving from left to right. The line shown is the calculated trajectory of the sphere.*

Table 1 The error of the translation test

Interface	CFL	E
Sphere	0.414	1.24×10^{-2}

3.1 Translation

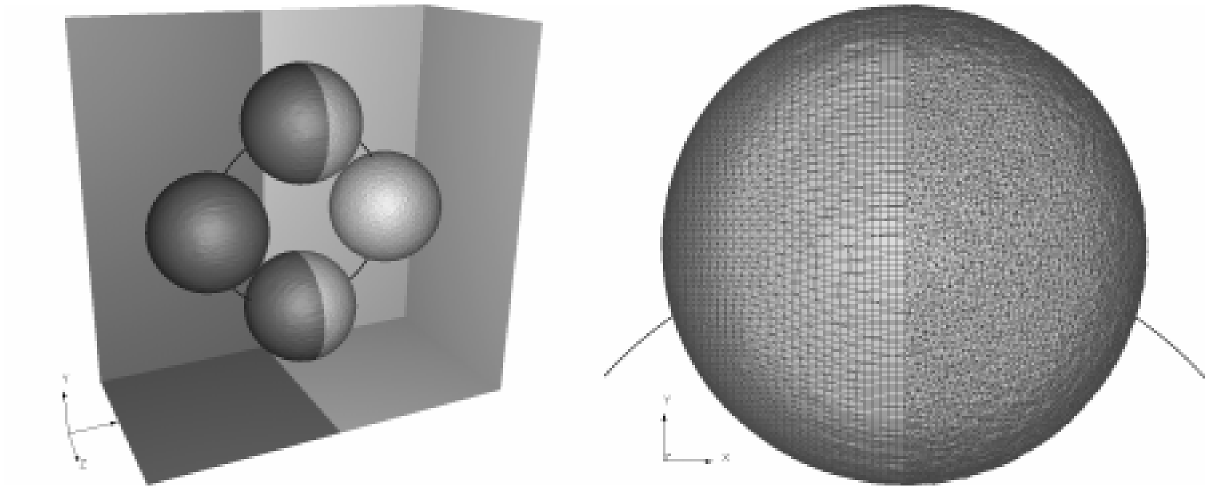
The domain used in this test is a cube of which length L of each edge is equal to unity. We use a hybrid mesh composed of tetrahedral and prism cells. There exist prism cells in width of $0.3L$ from each end-face in x-direction, as shown in Figure 3, while usually prism cells are used towards walls in boundary layers. Typical width h of cells used is $0.02L$. The shape of the interface is a sphere of which radius R is $0.15L$. Hence $2R/h$=15. The initial position of the centre is (0.25, 0.25, 0.25). The maximum Courant number is 0.41, which is not the maximum number in the whole domain but the maximum number in actual cells calculated.

The result is shown in Figure 4, which is the shape after moving distance $\sqrt{0.75}L$. The discritised equation (7) does not cause errors in translation tests. Therefore the error in this test is caused only by the reconstruction error of interfaces and does not depend on the Courant number used if the number is equal to or less than 1. The error is shown in Table 1.

3.2 Rigid-body rotation

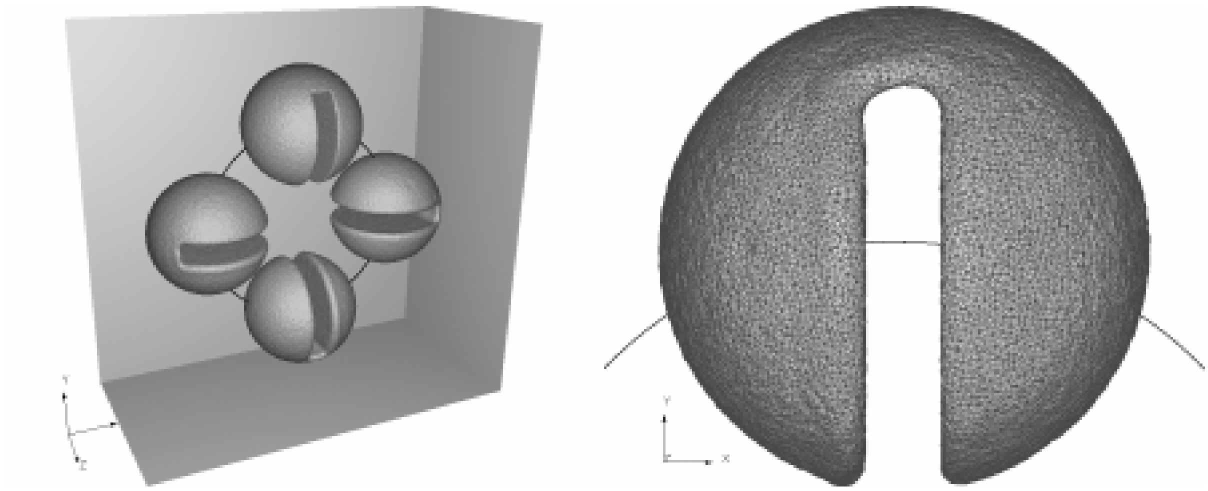
The domain used in the rigid-body rotation test is $x\times y\times z = L\times L\times 0.5L$, where L is unity. Two types of meshes are used. One of them is composed of prism and tetrahedral cells of which boundaries exist at x=$0.5L$. The other is composed of tetrahedral cells only. Typical width h of cells used is $0.005L$. Two types of the interface, a sphere of which radius R is $0.15L$ and a sphere with the slot of width $R/3$ and length $5R/3$, are used. Hence $2R/h$=60. The initial centre position of each sphere is (0.5, 0.75, 0.5). The rotation is provided around z axis.

The errors are shown in Table 2. As the slotted sphere has large curvatures at the corner of the slot which are too severe to reconstruct interfaces accurately, the errors of the slotted sphere on both meshes are greater than those of the sphere and largely caused by the reconstruction error of the interfaces. The errors on mesh composed of tetrahedral cells only are also smaller than those of the other, since typical width of both meshes used is the same but spatial resolution of tetrahedral cells is higher than that of prism cells. Figure 5 and 6 show the shapes of the interface within one revolution.



(a) *Time series of the revolution* (b) *After one revolution*

Fig. 5 *The results of rotation test of the sphere on mesh composed of prism and tetrahedral cells. The line shown is the calculated trajectory of the slotted sphere. The direction of the rotation is counterclockwise in this view. The sphere goes through prism (dark) and tetrahedral (bright) cells.*

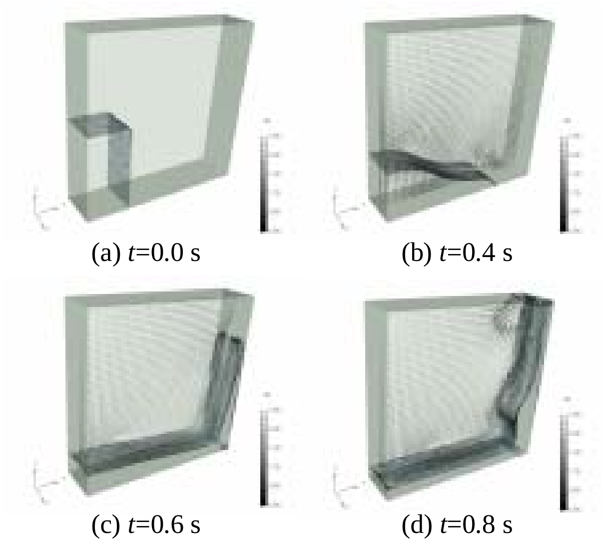


(a) *Time series of the revolution* (b) *After one revolution*

Fig. 6 *The results of rotation test of the slotted sphere on mesh composed of tetrahedral cells only. The line shown is the calculated trajectory of the slotted sphere. The direction of the rotation is counterclockwise in this view.*

Table 2 The errors of the rotation test

Interface	Mesh	CFL	E
Sphere	Prism & Tetra	0.491	1.01×10^{-2}
Sphere	Tetra	0.504	9.37×10^{-3}
Slotted	Prism & Tetra	0.491	3.47×10^{-2}
Slotted	Tetra	0.504	2.57×10^{-2}



(a) t=0.0 s (b) t=0.4 s (c) t=0.6 s (d) t=0.8 s

Fig. 7 *The result of the broken-dam.*

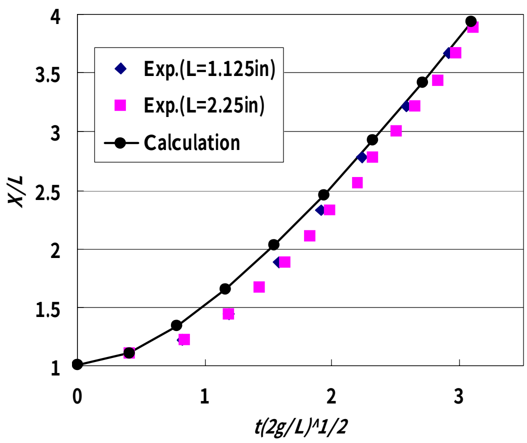


Fig. 8 *The comparison of the leading front.*

3.3 The Broken-dam problem

The domain size is $x \times y \times z = 4L \times 4L \times L$ and L=0.146 m length. The initial water column is located in the size of $L \times 2L \times L$. An opponent medium is air. Surface tension was taken into account by CSF (Continuum Surface Force) model [4]. Mesh used is composed of tetrahedral and prism cells and the numbers of cells and nodes are 399911 cells and 84860 nodes, respectively. The Courant number for calculating the advection equation was set up to 0.5 throughout this calculation.

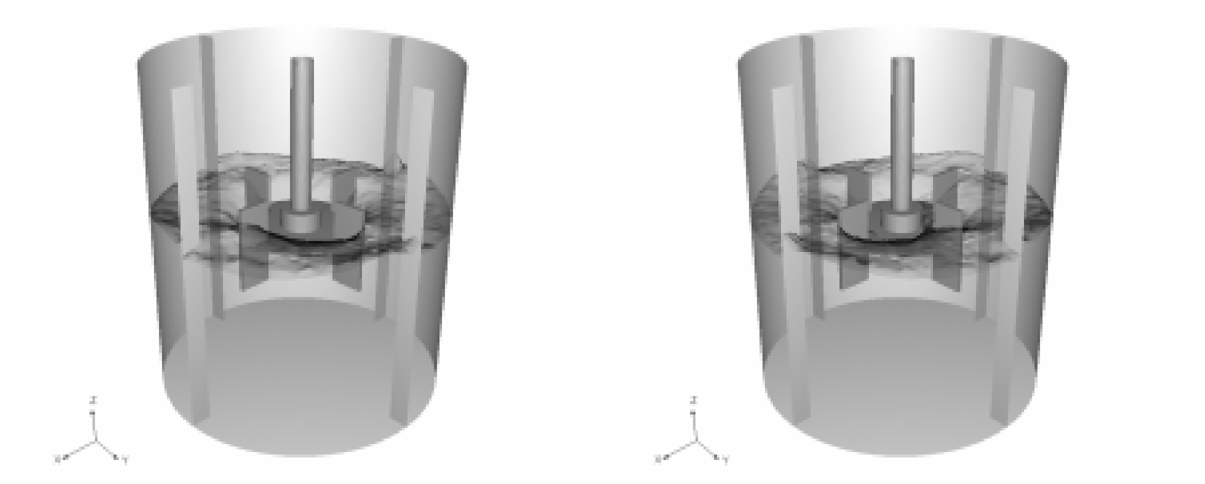
The proposed advection scheme was incorporated into SC/Tetra (Software Cradle Co., Ltd.), which is a general purpose solver for fluid flows using hybrid unstructured meshes, including an auto mesh generator and a post processor. In SC/Tetra, the governing equations are discritised by the finite volume method and SIMPLEC method is used for coupling between the continuity of incompressible fluids and pressure. This calculation was performed on 8 computers in parallel.

Figure 7 shows time sequence of the free-surfaces and velocity vectors in the domain. The currents are induced by the pressure differences due to the gravity. Thus the column of water collapses and then breaking-up and merging of the free-surface occur. The leading front of the free-surface in this process until the free-surface reached the vertical wall is shown in Figure 8. The calculation result is reasonable agreement with the experimental ones [5].

4. A TURBULENT FLOW WITH FREE-SURFACE IN A STIRRED VESSEL

The impeller used is the Rushton turbine of which diameter and width are 0.076 m and 0.04 m, respectively. Diameter and height of the vessel are 0.14 m and 0.16 m, respectively. The number of baffles is 4 and its width is 0.01 m. Height of the impeller from the bottom of the vessel is 0.08 m. Height of free-surface from the bottom is set up at 0.09 m. The working fluids are water and air. The number of revolution is 100 rpm and the direction of the rotation varies every 2 seconds periodically.

In order to calculate this flow, ALE (arbitrary Lagrangian-Eulerian) method was used. The whole domain in the vessel is taken apart to two domains. One of them is rotational part, which moves according to the movement of the impeller. The other is static part. Therefore there exist discontinuous boundaries between meshes of those parts. In the proposed scheme, there is no need to modify its formulation and discritisation for the discontinuous boundaries



(a) t=4.75 s (b) t=6.75 s

Fig. 9 *The free-surfaces in the stirred vessel. (a) shows during counterclockwise rotation and (b) during clockwise rotation in the top view.*

as well as SC/Tetra can deal with those ones properly. The standard k-ε model was also used for analysing a turbulent flow. This calculation was performed on 16 computers in parallel using mesh composed of tetrahedral and prism cells of which the number of cells and nodes are 156723 cells and 41864 nodes, respectively. It is found that the proposed scheme can calculate the volume fraction of a fluid without losing of the accuracy despite of the fact that there exist discontinuous boundaries in mesh used, as shown in Figure 9.

5. CONCLUSION

An advection scheme for using the Lagrangian remap was proposed and the results of some calculations were shown in this paper. It was revealed that the proposed scheme has the following characteristics.

(1) It does not need any procedures out of its formulation for correcting overestimation and underestimation of transported volumes induced by incomplete formulation in the discritised advection equation.
(2) It can be used on arbitrary meshes composed of any polyhedron even if there exist discontinuous boundaries in mesh used.
(3) It is stable and robust if the Courant number is only equal to or less than 1.

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