ALICE: AN ARBITRARY LAGRANGIAN-EULERIAN CODE FOR ANALYZING CONTAINMENT RESPONSE TO HCDA

by

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Summary

This paper describes a reactor containment code, ALICE (Arbitrary Lagrangian-Eulerian Implicit-Explicit Containment Excursion code), which is developed at Argonne National Laboratory. The code uses a hybrid Lagrangian-Eulerian finite-difference method for the treatment of the coolant motions and a Lagrangian finite-element technique for the analysis of the containment vessel and other solid media inside a reactor containment.

The advantages of the ALICE code over the conventional Lagrangian or Eulerian method are: (1) the interpolations of the fluid and structural motions can be made very accurate as the cell vertices of the fluid adjacent to the structure moving with the structural nodal points; (2) the cells for the fluid calculation can be made in any quadrilateral shape corresponding to the perforated passageways or the structural deformation to avoid irregular-cell calculations; (3) inlet and outlet boundary conditions can be easily treated; (4) long-duration calculations can be achieved by rezoning the large distortion regions; and (5) a pure Lagrangian approach can be applied to those small distortion regions to treat flow problems with many materials.

Numerical calculations for the fluid solution are separated into three phases. The first phase consists of an explicit Lagrangian calculation. The second phase, which is optional, contains an implicit iteration. The third pase, which is also optional, rezones the mesh vertices to the prescribed positions.

There are two structural elements used for the ALICE analysis. The first one is a shell element which uses the large-displacement small-strain theory. Each shell element associates with a set of corotational coordinates. The second element is a quadrilateral solid element. The equations of motion for this element are formulated through the use of intermediate nodal forces.

Both explicit-explicit and implicit-explicit coupling calculations for the fluid and structure can be performed by the ALICE code. The calculations are implemented into two separated steps. The fluid supplies the structure with a pressure loading which causes the motion of the structure. In return, the structure gives the fluid a moving boundary condition at the fluid-structure interface.

Two examples are given to illustrate the application of the ALICE code. The first one is a shock tube test in which an initial discontinuity of pressure and density is calculated. The second one is a SRI flexible-vessel test specially designed for the containment code validation. Results are discussed in detail.

1. Introduction

The advancement of the digital computer made it possible to use the numerical method for solving non-linear fluid-structure interaction problems in a reactor containment system. Since the first introduction of the REXCO code [1] in 1969, a great number of containment codes have been developed and reported in the literature. However, all of those codes use either Lagrangian [2,3] or Eulerian coordinates [4,5] for the description of the fluid motion.

In the Lagrangian approach, the mesh used to describe the fluid motion moves with the fluid. Difficulties arise when the physical system involves slip surfaces, large mesh distortion, and inflow and outflow boundary conditions. In the Eulerian approach, on the other hand, the mesh used to describe the fluid motion is fixed in space. Although such mesh is ideal for treating excessive fluid distortions, difficulties also arise when the physical system involves material interfaces and moving structural boundaries.

To overcome the limitations associated with a pure Lagrangian or Eulerian method, a two-dimensional code, ALICE (Arbitrary Lagrangian-Eulerian Implicit-Explicit Containment Excursion code) [6], is being developed at the Argonne National Laboratory (ANL). The code uses a finite-difference arbitrary Lagrangian-Eulerian approach as given by Hirt et al. [7] for the description of the fluid motion and a finite-element Lagrangian method for the analysis of the structural response. These two calculations are coupled in such a way that the fluid supplies the structure with a pressure load and the structure gives the fluid a moving boundary condition.

Since the vertices of the fluid cells adjacent to the structure can always be moved to coincide with the structural nodal points, no special treatment for irregular cells is needed and the computational procedure is greatly simplified. The interpolations of the fluid and structural boundary conditions can also be made very accurate. The basic methodology used to solve the fluid and structures is briefly described in Section II. Section III gives two examples to illustrate the present capability of the code.

2. Methodology

2.1 Fluids

To solve the conservation equations for the fluids with a numerical method, the physical system is discretized into a number of quadrilateral cells. The vertices of these cells are designated by a pair of integers (i,j) with i counting from left to right and j from bottom to top (see Fig. 1). Fluid variables such as pressure, density, specific total energy, specific internal energy, volume, and mass are assigned to the cell center $(i+\frac{1}{2},j+\frac{1}{2})$; whereas coordinates and velocity components are assigned at the vertices. Initial and boundary conditions are set through the use of input data to this discretized system to start the calculation of a problem.

Fluid calculations to advance a solution one step in time are separated into three phases. The first phase consists of an explicit Lagrangian calculation. Velocities are advanced by the pressure gradients, inertia forces and viscous forces. Energy changes due to inertia and viscous forces are also calculated in this phase. The energy change due to the pressure work will be performed after the second phase to permit using advanced-time pressures in computing work to coincide with the advanced-time velocities.

The second phase performs an implicit calculation. The basic task of this calculation is to eliminate the Courant stability condition which limits the pressure waves to travel over one cell per time step. A Newton-Raphson iteration method is used to obtain advanced-time pressures which in turn are calculated by the discrepancies of the transport equations. Fol-

lowing the pressure changes at each iteration, densities, specific internal energies, and velocities are also adjusted. The converged pressures are used for the calculation of the pressure works to update the energy changes.

If at this point of calculation, the mesh vertices are moved with the fluid, the result is Lagrangian. It is well known that the Lagrangian solutions are not accurate when the computing mesh is severely distorted. To avoid large mesh distortion and maintain an optimum mesh, the third phase performs a rezone calculation which allows the computing mesh to move in a prescribed manner. Convective fluxes due to the relative motions between the computing mesh and fluid are calculated to assure the conservations of mass, energy and momentum.

Marker particles are used to trace the location of the free surfaces and aid in visualization. They are moved by local fluid velocities. Once the locations of the free surfaces are found, free-stress conditions are imposed to the surface fluid cells to calculate the fluid motion.

2.2 Structures

Structural calculation uses the Lagrangian approach because of the strong history dependence of the structural constitutive equations. At present, two types of elements, elastic-plastic solid media and shell elements, are used in the ALICE code. The original calculation of the solid media uses the finite-difference formulation as given in Ref. [2]. To facilitate the treatment of the boundary conditions and the arbitrary combination of the solid media, the fluid, and the shell structures, the equations of motion for the solid media are formulated through the use of intermediate forces. Thus, the equations of motion for both solid media and shell elements can be written as

$$M\ddot{u} = F^{ext} - F^{int} , \qquad (1)$$

where M is the generalized mass matrix; u the generalized displacements; F^{ext} the generalized external forces; and F^{int} the generalized internal forces. The dots over the quantity denote time derivative of that quantity. The generalized external forces are calculated from the pressure loadings given by the fluid. Nonlinearities in material properties are approximated by a multilinear stress-strain relations. Equations of motion are explicitly integrated in time using a central difference approach.

The solid element is quadrilateral in shape. The mass at each nodal point is calculated by the contribution of the masses from its four adjacent elements. Deviator stresses are computed from the incremental strains and volumes. The von Mises yield criterion is used for the determination of those deviator stresses whether they are in the elastic or plastic region. If the computed deviator stresses exceed the elastic region, they must be reduced by a factor to calculate the generalized internal forces.

The thin shell element uses a corotational coordinate. Rotation of the corotational coordinates associated with each element is represented by the rotation of the line connecting its two nodal points. Masses at each nodal point are determined in such a way that the translational and rotational inertia are, respectively, equivalent to the mass and mass moment of the segment between the nodal point and the midpoint of the element. Large displacements are entirely contributed by the rigid body rotation of the element. In the corotational coordinates, the deformation displacements are small. The displacements are linearly related to the strain and the nodal forces are linearly related to the stresses in the corotational coordinates. Thus, a very efficient computation can be performed in the calculation. De-

tails of the formulation are given in Ref. [8].

2.3 Fluid-Structure Interaction

As mentioned earlier, the fluid uses an arbitrary Lagrangian-Eulerian mesh with either implicit or explicit time intergration; whereas the structure uses a Lagrangian mesh with only explicit time integration. Thus, both implicit-explicit and explicit-explicit coupling calculations can be performed by using the ALICE code. The calculations for the fluid-structure interactions are implemented into two separated programs and interconnected only through normal input and output subroutines.

The fluid pressures at time t are used to calculate the locations and velocities of the structures at time $t + \Delta t$. The velocities of the structures at time $t + \Delta t$ are then given to the fluids as the moving boundary conditions. At the fluid-structure interfaces, the fluid can slide freely along the structural surfaces, but must be moved together with the structures in the normal direction.

Stability conditions are separately imposed on the fluid and structure due to their large differences in the frequency content. For explicit-explicit coupling calculation, the same time step may be used for both fluid and structures. But for implicit-explicit coupling calculation, several time steps are usually performed in the structural analysis to match one time step of the fluid in order to save the computational time.

The optimum choice of the mesh movement for the fluid-structure interaction problems is that the vertices of the fluid cells adjacent to a structure move with that structure. Thus, the movement of the structure relatively to the fixed space will not create any irregular cells for the fluid calculation. To achieve this goal, vertices of the fluid cells moved by the Lagrangian calculation must be rezoned to match the locations of the structural nodal points. Convective terms are calculated for this relative motion to assure the conservations of mass, energy, and momentum.

3. Sample Problems

A variety of problems have been analyzed by the ALICE code, two of them are described and illustrated in this paper.

3.1 Shock Tube Test

The first example is a shock tube problem with an initial pressure and density discontinuity as given in Problem #1 of the APRICOT program [9]. The purpose of this example is to test the calculation of the motion in z (or y) direction and to check the variables calculation in r (or x) direction. Figure 2 shows the configuration of the shock tube that has a rigid tube wall and two rigid end caps and is divided into two gas regions by a diaphragm. At time $t = 0$, the diaphragm is removed. A shock wave initiated at the interface is propagated toward the right side, while a rarefaction wave moves in the opposite direction.

Since the ALICE code can solve this type of problem in either the Lagrangian or Eulerian method using either the explicit or implicit integration scheme, several calculations have been performed. Results of the pressure profile for the explicit Lagrangian calculation without artificial viscosity shows that spurious oscillations are generated as the pressure waves travel in both directions. To prevent this, two types of artificial viscosities are used in the ALICE code to spread the shock calculation so that the conservation equations can be solved without discontinuities. One is the Von Neumann-Richtmyer viscosity A_q, which is quadratic in the dilatation rate, and the other is Landshoff viscosity A_ℓ, which is linear in the dilatation rate. The values of $A_q = 3.0$ and $A_\ell = 0.05$ seem to provide adequate damping

for eliminating the spurious oscillations as shown in Fig. 3. However, a Von Neumann-Richtmyer overshoot has still appeared at the rarefaction wave front, and some small numerical noises still exist in the portion between the shock and rarefaction wave fronts.

Although no artificial viscosities were used for the Eulerian calculation, the Eulerian results were smoother than the Lagrangian counterpart (see Fig. 4). The Eulerian solution produced an overshoot at the shock wave, but no overshoot can be seen at the rarefaction. Not only is the wave profile very smooth, but the wave front is also very sharp and distinct.

Both the Lagrangian and Eulerian results calculated by the ALICE code are in excellent agreement with the analytical solution. An implicit integration calculation was also performed with the ALICE code. Spurious oscillations have been virtually eliminated from the numerical calculations.

3.2 The SRI Flexible-Vessel Test

The second example compares the ALICE code predictions with the SRI flexible-vessel Tests FV101 and FV102 [10]. These tests were designed and performed for the validation of the containment codes.

The test configuration for Test FV101 is shown in Fig. 5. The cylindrical vessel wall was made from annealed Ni-200 material which simulated the same mechanical properties of Type 304 stainless steel at reactor operating temperature. The cylindrical core barrel was made of 2.54-cm-thick steel. Test FV102 had the same configuration as FV101, except that the core barrel was made of a 2.413-cm-thick aluminum cylindrical shell. A Mylar diaphragm was placed on the core barrel 7.62-cm above the platform to prevent water from entering the initial air space of the energy source.

In the ALICE analysis, the physical system is discretized into 8 x 21 quadrilateral meshes. For Test FV101, the core barrel was modeled as a rigid obstacle, whereas in Test FV102, it was modeled as a continuum material having the properties of lead and combined with a flexible aluminum thin shell.

In both calculations, the code assumed that all the mesh vertices associated with a structure moved with this structure, and all the other vertices were fixed in space. Therefore, the deformation of the structure can be determined from the movement of the fluid grid lines. Fig. 6 shows the vessel configuration for Test FV102 at 1.2 ms after the start of computation. The deformation of the core barrel and vessel wall can be seen from the radial movement of the grid lines which were originally vertical and passing through the core barrel and vessel wall.

In general, all the pressure loadings and impulses calculated with the ALICE code are in good agreement with the experimental results. Gauges P8 and P9 were mounted on the cover to record the impact pressures. The magnitudes of the impact pressures, the wave arrival times, and the shapes of the pressure loadings at both gauges as calculated by the code agree very well with the experimental data, except the second pressure spike which appeared at gauge P8 in both experiments (at time 1.2 msec) was not predicted in the code calculations. This spike was believed to be caused by a second impact of the water surface after it had separated from the cover head immediately following the first impact. Since no surface separation after impact was allowed in the ALICE analysis, the computed results at P8 did not have the second spike; instead, it had a long duration of pressure loading with a lower magnitude.

The pressure loadings on the platform (P4) and vessel wall (P5, P6, and P7) are also in close agreement with the experimental results. Due to the space limitation, only the pressure histories at P7 for Test FV102 are given in Fig. 7.

Fig. 8 shows the respective profiles of the calculated wall and core barrel deformations for FV102 together with experimental measurements. The agreement between ALICE predictions and experimental results is exceptionally good, particularly for Test FV102. Not only are the vessel deformations in good agreement, but also the core-barrel deformations are in close agreement. For Test FV101, the core barrel was assumed to be a rigid obstacle. As a result, more energy was directed to the upper part of the vessel wall, thus causing more wall deformation at the upper vessel wall.

4. Conclusions

The development of the ALICE code has eliminated limitations associated with a pure Lagrangian or Eulerian solution. Thus, it can be effectively applied to a large variety of safety problems found in a reactor containment system.

As illustrated in the example problems, the ALICE code predictions have been compared with a theoretical solution as well as the experimental results. Good agreement indicates that the ALICE code is an essential tool to analyze containment response during a hypothetical core disruptive accident (HCDA).

5. Acknowledgments

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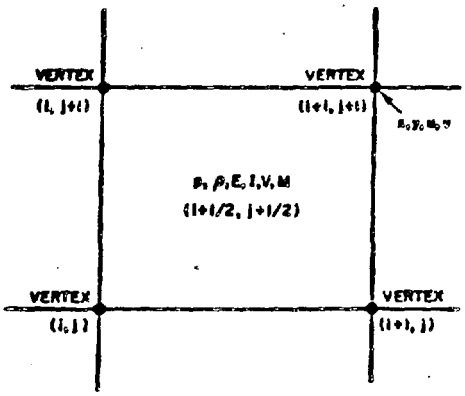

Fig. 1. Field Variable Placement in a Typical Cell.

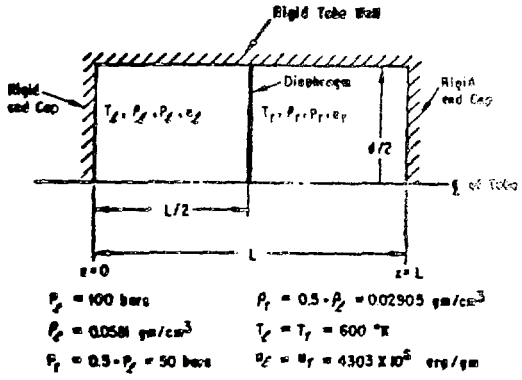

Fig. 2. Schematic of Tube (not to scale).

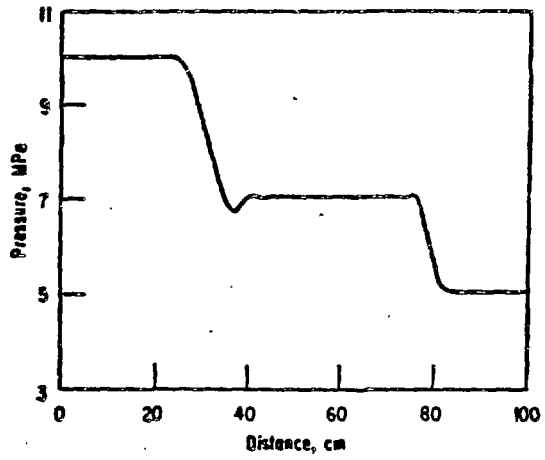

Fig. 3. Pressure Profile at 500 μs (Lagrangian).

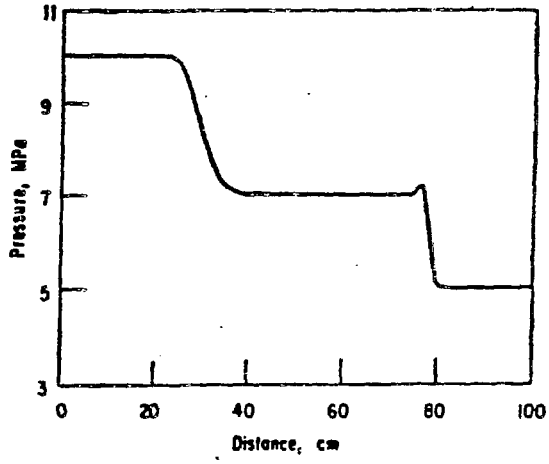

Fig. 4. Pressure Profile at 500 μs (Eulerian).

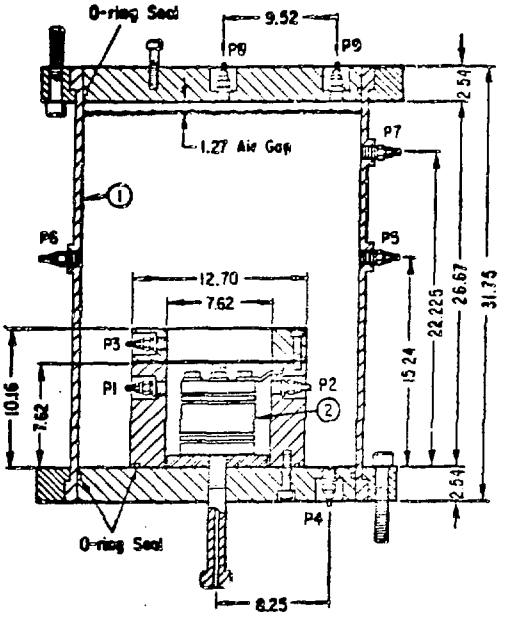

Fig. 5. Test Modal for FV101.

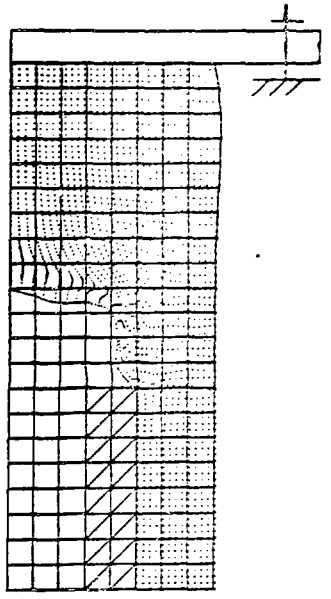

Fig. 6. Vessel Configurations for FV102 at 1.2 ms.

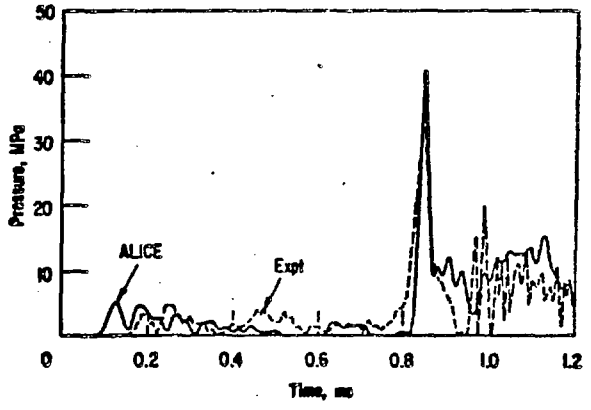

Fig. 7. Pressure Histories at P7 for FV102.

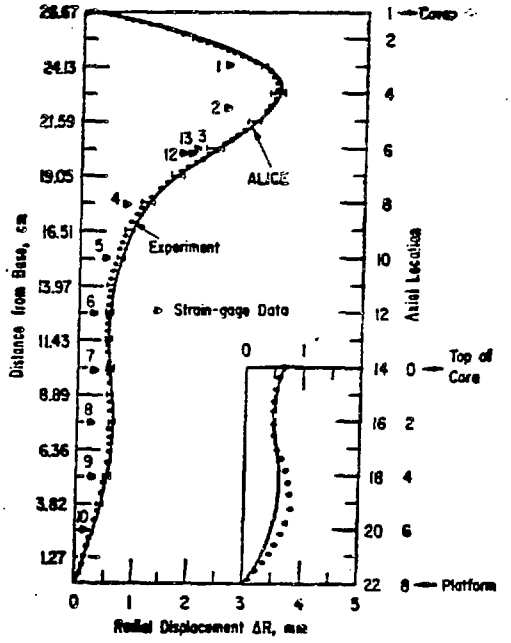

Fig. 8. Permanent Vessel Deformation for FV102.