AN EULERIAN STUDY OF PROPAGATION OF FAST REACTOR EXCURSION*

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ABSTRACT

An Eulerian method specifically designed to study the propagation of fast reactor excursions and their effects on the surroundings is described. The method is based on what has been referred to as the Particle-in-Cell (PIC) technique. A provision of a solid boundary, which is able to move under an imposed pressure, is incorporated into the procedure. Comparison of sample results is made with those obtained by means of a corresponding Lagrangian solution. A simulated plug-jump problem is illustrated and the encountered difficulties described. The capability of monitoring possible coolant spillage to the outside of primary containment by means of the proposed method is pictorially illustrated and discussed.

1. INTRODUCTION

Knowledge of all effects resulting from the entire duration of a given fast (high-energy) excursion is important in reactor design. A typical fast excursion and the realization of its destructive potential may be a matter of a fraction of a second, which is a very long time in the study of explosions. During this time the character of the excursion would change continuously; first, a shock wave may appear, this taking place within microseconds. Reflected waves within the containment system would then follow. A mixture of these waves would prevail for some time until their final dissipation.

In turn, when the fluid is accelerated by the passage of the waves it gains in velocity and progressively imposes its effects on the surroundings. The influence of fluid momentum should make itself known within the time of milliseconds. This state of the fluid would be characterized by pressure perturbations and corresponding reactions of the containment structure, until equilibrium of the system would come into play. In this equilibrium state the full effect of residual core pressure would be directly balanced by the containment structure.

The course of a typical fast excursion would thus encompass practically the entire spectrum of fluid flow. In certain situations the fluid may be regarded as incompressible, and in others its compressibility may play a very important role. Sometimes the state of the

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fluid may be characterized by excessive deformation, while at other times deformations may be small. There are instances where the effect of heat transfer may be negligible, but in other cases this effect may be predominant.

The presently available analytical tools in hydrodynamics are unable to include all the relevant variables coming into play during the entire course of the fast reactor excursion. Hence, in order to make use of the available techniques in the containment study, certain simplifying assumptions must be made. In this sense the effect of important variables would be enhanced, while those of others suppressed, or neglected altogether. In fact, the entire treatment must necessarily be subdivided into parts; different tools, emphasizing distinct flow characteristics, would then apply to only certain delineable segments of the excursion.

One very effective tool in the study of fast reactor containment has been the REXCO-H computer code described by Chang et al. [1]. This Lagrangian code is ideal for treating compressible flows of the excursion, where the effect of shock waves needs to be investigated. Information on fluid momentum in relation with the immediate primary containment is also obtained. Additional data can be inferred from the results of REXCO-H solution to judge on the subsequent behavior of the containment unit. Excessive deformation of the fluid and thus the assumed Lagrangian grid, however, forces termination of the REXCO-H solution before the entire duration of the excursion can be examined satisfactorily. The application of this code to a typical containment problem could possibly be extended to a period of as much as one hundred milliseconds of the excursion.

The REXCO-H code provides a reasonable description of the containment solution for only a fraction of the excursion time. With the intention of prolonging the study period of the excursion, other analytical tools in hydrodynamics were also sought. This paper provides an account of the search of and experience with another method of analysis.

2. CONSTRUCTION OF THE EULERIAN PROCEDURE

In order to follow the progress of the excursion during the subsequent time period, consideration was given to the utilization of other tools, and particularly the Eulerian methods of analysis. With the Eulerian approach the treatment of excessive deformations would only be natural, which is not the case with the Lagrangian method. In order to utilize both methods most effectively the study of a given excursion would be conducted by using the Lagrangian method for the initial stages, up to the time of excessive grid deformation; after the point of termination, the solution would then continue by means of the Eulerian method. This approach would effectively utilize the advantages of both methods. However, transformation of the Lagrangian variables into those of the Eulerian procedure would be needed, and this preferably in an automatic manner. Such a symmetric transformation could only be sought by knowing in advance the specific Eulerian method to be used.

An Eulerian technique called PIC (Particle-in-Cell), as described by Amsden [2], had proved its usefulness in solving a wide variety of problems involving the dynamics of compressible fluids. This Eulerian method also appeared to be the only one available at that time which was adapted for analysis of multimaterial fluids. One of its basic disadvantages, the quantized character of the method, may also be used here to advantage in another sense: the fluid particles may provide a means for carrying heat in a particular nuclear excursion.

In addition, it appeared as if this approach could be adapted to the containment problem without too much difficulty.

2.1 TRANSFORMATION OF INPUT VARIABLES

The first step of the overall effort was the task of accepting the output of the available Lagrangian REXCO-H code at the instant of termination and converting this information into such form as would be needed for the input of the Eulerian-coordinate solution. Consequently, the computer program called TRANSF was written to accomplish this operation.

Basically, this computer program converts a volume of a given material into a chosen number of particles per unit of initial grid area of the Lagrangian mesh. The program then divides the deformed individual Lagrangian grid area into as many equal portions as there are particles and assigns them to their respective centroids. Concurrently, each particle is also given the properties of the original Lagrangian mesh. A chosen Eulerian grid is then superimposed on the various particles established previously. Location of the particles within the Eulerian grid is noted and the particles are labeled accordingly. Properties of the individual Eulerian grid are finally determined by averaging the particle properties within each grid.

Thus, relevant variables from the Lagrangian output at a predetermined time are systematically transformed into the input for the PIC routine. A sample of the deformed Lagrangian grid and a corresponding Eulerian particle distribution is shown in fig. 1. Different symbols of the Eulerian representation pertain to different materials of the reactor model.

2.2 MODIFICATION OF THE EULERIAN PROCEDURE

The computer code using the PIC technique is designed around a cylindrical configuration shown in fig. 2. Outside dimensions of the model are preassigned the rigid free-slip boundary condition. The model configuration is provided with a reactor cover which acts similar to a piston under the action of an unbalanced force. All dimensions and the sizes of the cells can be assigned values at will. The name REXCO-P is given to this computer code, meaning REactor EXcursion COde using the PIC method. The computer program uses the Fortran IV computer language and is particularly adapted for the IBM-360 computer.

The construction of the computer code was based on the outline given by Amsden. Although the mechanics of the code could be different in many respects, the methology followed was the same. Since the particulars of the PIC technique have been widely described in numerous publications, no mention of the details will be made here; described will only be the deviations from the PIC technique.

One major addition to the regular PIC procedure in the REXCO-P code is the incorporation of a movable boundary condition. This boundary condition is rather simple in principle: an entire segment of a given boundary, when subjected to internal pressure, may be permitted to move. This motion or displacement would be the same for the entire segment of the boundary.

The movable boundary introduces a variable-size Eulerian cell, the magnitude of which depends on the total force acting on the whole movable segment. Of particular concern here is the instance when the Eulerian cell underneath the plug is so small that no fluid

particles have as yet moved into it. The pressure in this cell can hardly be taken as zero as called for by the PIC technique. If this is done, the adjacent fluid will then be assigned an excessive acceleration in the direction of the plug. In the subsequent time increment of the solution fluid particles may already enter into the cell. Then, due to the small volume of the cell, the pressure calculated may be very large. This sudden increase in pressure would tend to act like a discontinuity, adding considerably to the unstable conditions at the movable boundary.

To remedy this situation, pressure in a newly formed cell is determined by considering fluid particles within a specified distance from the plug boundary. This distance, although somewhat arbitrary, may become quite dominant in the success of the technique. If this distance is taken to be considerably smaller than the height of the Eulerian cell, then the density of the fluid and hence the respective pressure within the volume may become very large. On the other hand, at the time of separation of the fluid from the plug, this distance should be as small as possible. Otherwise, even if separation had already taken place, the fluid within the given distance would still exert its influence on the plug.

As a consequence, the technique incorporated into the Eulerian code separates this boundary pressure calculation into two parts: one, pertaining to the pressure acting on the plug, and two, pertaining to the pressure assigned to the adjacent cell of the boundary. The fluid particles which are assumed active in displacing the boundary are those within one-half the Eulerian cell height from the boundary. All these particles are collected and the corresponding pressure calculated. With the pressure at the boundary known, the velocity of the plug is computed, subject to prescribed and supposedly known restraints. Assuming this velocity to be constant during the given time increment, the displacement of the boundary follows. This then establishes the size of the Eulerian cell next to the boundary; the size of the cell remains unchanged through the subsequent calculations within the given time-cycle.

The pressure assigned to the cell adjacent to the movable boundary is obtained similarly, except that fluid particles within one full height of the Eulerian cell are taken into account. This pressure is consequently used for transport of the fluid particles.

The procedure in determining the pressure adjacent to the movable boundary is somewhat arbitrary. Although different approaches have also been attempted, the procedure described above appears to yield the best results so far. Provision of the movable boundary condition, coupled with the assumed geometry and the free surface boundary, provides the means for the consideration of fluid spillage.

3. COMPARISON OF SAMPLE RESULTS

The comparison here is based on a simplified pancake-shaped reactor model. The model consists only of a core and coolant, the initial configuration of which is shown in fig. 3. For purposes of comparison only one-fourth of the axisymmetrical reactor is considered in the model. The left centerline corresponds to the center axis of the cylindrical reactor, while the bottom boundary corresponds to the central horizontal plane dividing the core into half. The coolant in fig. 3 is shown by means of dots.

All the boundaries of the model are assumed to be ideally rigid with no resistance to slip. In addition, the movable boundary provision is not utilized; the plug is taken to be rigidly fixed.

The initial conditions of this example are taken from the power-excursion calculation, a separate analysis, which takes the neutronics of the excursion into account. It is assumed here that at the start of this problem the neutronics have ceased and the core consists entirely of a gassified oxide core. The condition is such that the core behavior can now be represented by an equation of state, and the outside boundaries of the core have not as yet moved. The input conditions of the Lagrangian code are transformed for the Eulerian code by way of the TRANSF routine. Four Eulerian particles are assigned to each of the Lagrangian cells of the coolant and sixteen particles to that of the core. The height and width of the Eulerian cells are made twice larger than those of the undeformed Lagrangian cells. Consequently, at the beginning each Eulerian coolant cell contains sixteen symmetrically positioned particles and each core cell contains sixty-four particles.

The initial pressure and internal energy on the centerline of the model is displayed in fig. 4, where the first two cells pertain to the core and the rest to the coolant. These initial conditions are identical for the first eight columns of the model; those of columns nine and ten are also shown in fig. 4. Initial velocities of both the coolant and the core are taken as zero.

The solution of the example problem by means of the REXCO-P code is run with a constant time increment ($\Delta t = 0.000004$ sec), which is within the limits of stability criteria for both the Lagrangian and the Eulerian solutions. This is done in order to facilitate a direct comparison between results obtained by both methods. Some results, yielded from the Eulerian solution, are displayed in fig. 5; these show configurations of the coolant at different periods in time.

Several representative cells are selected to display certain characteristics of the solution. These are indicated in fig. 3 and identified by numbers 1 through 4. The first point represents the conditions at the center of the core, and the second part is on the centerline of the reactor but on the boundary and within the coolant. Point three initially represents the radial outside edge on the core, and point four is located within the coolant at an asymmetrical location.

All the characteristics of the Eulerian solution so displayed are compared with the corresponding Lagrangian results. For this purpose the Lagrangian REXCO-H code was modified by incorporating into it the TRANSF routine. The object of the TRANSF code was to convert the Lagrangian results into the form of the Eulerian output without changing the Lagrangian method of solution. In effect this modification would cause a superposition of the Eulerian mesh over that of the Lagrangian at specified time intervals. The average of the Lagrangian properties within each Eulerian cell would then be calculated and given in printed output. Such an Eulerian output of the Lagrangian solution would thus provide a very convenient means for comparison. Consequently, a smooth curve in the subsequent illustrations represents the Lagrangian results while a block diagram portrays the Eulerian solution. This type of representation for the Eulerian results is used because of a rather large variation in properties from cell to cell and from one cycle of calculation to the next.

Fig. 6 shows the pressure history at locations 1 through 4 within one millisecond. This is a time span exhibiting the first pressure pulses on the boundary. The pressure at two

points within the core (location 1 and 3) do notably agree better with the Lagrangian solution than those within the coolant. One reason for this is the type of equation of state used, or rather the kind of material considered in the analysis. Actually, the pressure of the coolant depends to a small degree on the internal energy. Primarily, however, the stepwise Eulerian pressure distribution depends on the number of particles within the respective cells. The pressure of liquids (and solids) are naturally much more sensitive to changes in density. Even if the configurations of the pressures due to Eulerian and Lagrangian solutions do not quite coincide, the area underneath the curves, representing an associated force, appears to be fairly close.

The oscillations from cell to cell in pressure are also transmitted to the velocities. Radial and axial velocities of points 3 and 4 are illustrated in fig. 7. It is noted that location 4 is representative of a two-dimensional flow region. At this location the particle transport is expected to be more evenly distributed; consequently, the variation in properties at location 4 with time should not be as great. The result, however, is not noticeably different from the results in location 2.

The general trend of variations in pressures and velocities at the selected locations, due to the Eulerian and Lagrangian solutions, are comparable. Area under the respective curves or block diagrams is of the same magnitude if averaged over several cycles of calculation. When considered on an averaged basis, it appears that agreement in this rather restrictive sample calculation is not only qualitative but to a degree also quantitative.

Usually a good indication of the quality of the method of analysis in hydrodynamics is the degree to which it satisfies the conservation equations. The variation in the total energy of the REXCO-P solution is shown in fig. 8. Since this method does satisfy the conservation of energy rigorously, deviations do reflect the computer round-off errors, assuming that all attributing mistakes in the computer program have been eliminated.

The period of time used for the comparison of results is obviously very small. The model too is somewhat unrealistic with respect to the ideally rigid boundary conditions. So are also some of the input quantities used in the calculations. The intent of the sample problem, however, is the illustration of the performance of the technique rather than a very realistic description of the excursion effects. The fixed boundaries create conditions which effectively shorten the time of the excursion. This condition permits longer runs of the computer program.

4. THE PLUG-JUMP PROBLEM

In order to illustrate the performance of the plug movement, the reactor model shown in fig. 3 was used. Everything was assumed to be the same as in the previous sample problems, except the plug was permitted to move under the action of the increased coolant pressure. No other restraints against motion were specified, except the mass of the plug.

The results are displayed in fig. 9. This solution is particularly characterized by a noticeable oscillation of the fluid particles adjacent to the movable boundary. Undoubtedly this is due to the stepwise movement of the plug combined with a conditional particle reflection back from the boundary.

One particular difficulty in the movable boundary condition appears due to the formation of particle clusters. This takes place in the fluid impact situation where the boundary

is moving and the impinging particles are reflected back into the compressed flow region. The regular procedure may thus place the reflected particles over the adjacent particles, or may even project them farther back into the body of the oncoming flow. Once the coordinates of two or more particles are the same or nearly so, they both become inseparable from that point on. As a result, once the fluid has been "compressed" in this manner, the regular method of the analysis is unable to separate the distinct particles from one another.

Such a procedure of excessive reflection contradicts the physical behavior of the fluid in the impact situation. The obvious faulty mechanics of the technique is due to the complete freedom for the reflected particles to enter the interior of the fluid in the back. A remedial procedure should definitely restrain the reflected particles from passing the particles of the impinging fluid. In this way the integrity of the entire fluid body would be retained.

One possibility of correcting the procedural fault would be by devising a special reflective formulation in the fluid impact situation. Such a formulation would seek to render the particle overlap impossible, or at least decrease the probability. Some attempts in this line have already been made without a significant degree of success. Different particle weighting techniques may also be attempted. Another possibility of alleviating this difficulty may be the redistribution of particles whenever such an overlapping has taken place. This would be accomplished by subdividing the superimposed particles and positioning the new ones in opposite directions. Although this may offer some possibilities, it would not in itself help to eliminate the cause of the difficulty. Numerical techniques of the earch-type may always be utilized, but they would necessarily cost a considerable amount of computer time.

The performance of the assumed pressure boundary condition is again displayed by another illustration in fig. 10. In this case the number of particles of fluid in direct contact with the plug has been increased while still preserving the total mass. Instead of one previous particle, five have been created to represent the given volume of fluid. The particles were staggered in such a manner that equal distance between successive rows and columns was maintained. This increase in particles should reduce the total mass transfer from cell to cell at a given time thereby improving the stability of the solution. Pictorial results of fig. 10 clearly indicate the overlap problem which appears in the form of a band of particles below the plug.

The impact force on the moving boundary, or the plug, can be used to indicate the effectiveness of the increase in the number of particles. The total force on the reactor plug for the two cases, different only by the number of particles in the fluid layers adjacent to the moving boundaries, is shown in fig. 11. A considerable difference in the magnitude of the force is quite apparent, resulting in different displacements of the plug for the two cases. Difference in the plug movement may be noted by comparing figs. 9 and 10.

Further examination of this effect will need to be made to evaluate fully the consequences of the results. Remedies to the present techniques will be sought in order to make a reasonable solution of the impact problem possible.

5. SPILLAGE CONSIDERATION

Spillage of coolant to the outside of primary containment is illustrated by extending the plug-jump solution to a time when an assumed opening in the primary containment takes place. The results of the sample solution are displayed in fig. 12. The sample solution with the magnified number of particles is chosen for this purpose. This is done with the intention of providing a good pictorial illustration. Naturally, the greater the number of particles, the finer will be the resolution of coolant spillage.

The perturbation of the coolant displayed by fig. 10 is a subject of some concern. Apparently, this part of the solution is not quite correct. Although the corresponding quantitative results are not to be relied on, the illustrations serve well in displaying coolant spillage. Continuous inventory of the fluid mass spilled can easily be maintained in the code by monitoring the particles crossing a given opening.

The study of fluid spillage is dependent on the size of the individual particles. Since each particle is associated with a certain quantity of mass, the spillage would consequently be of quantized nature. Greater accuracy of the quantity spilled cannot possibly be resolved from this situation than is the mass of these individual particles. In order to get the required accuracy a certain modification of standard procedure may be needed. This may require another subdivision of already present particles adjacent to the spillage area into a greater number while preserving the total mass. The time of such a procedure should be just before the impending opening of the primary containment.

6. FINAL REMARKS

The superficial comparison of the Eulerian and Lagrangian results indicates agreement up to a point. Pressure and velocity magnitudes at selected locations, when considered on an averaged basis, do agree reasonably well when compared with results from a Lagrangian solution. It would appear that final results of the Eulerian code, when advanced in time, should produce reasonable load characteristics on the containment.

The considerable variation in magnitude of the plug force due to the change in the number of fluid particles, as exhibited in fig. 11, demands greater attention. According to the regular PIC procedure, change in the number of particles within a given Eulerian cell should only vary the degree of perturbation of the solution; it should not affect the end result to a noticeable degree. The fact that the results do not follow this reasoning brings forth the realization that the impact procedure is not as yet sufficiently well understood. More effort will be required in this area to better appreciate the implications emanating from the sample results.

The standard stability criteria specified in reference [2] do not seem to be sufficiently restrictive to containment problems. This is especially evident by observing the perturbations of the coolant in fig. 12. Thus, if the remedial procedures would impose an even finer time increment on the method, and this appears a very likely assumption, then the time element of the Eulerian code will become a serious disadvantage. Even now, when identical time increments are used in the Eulerian and Lagrangian codes, the Eulerian solution consumes approximately twice as much computer time as compared to that of the Lagrangian solution.

Correction of the particle superposition in the fluid impact situation should also expend additional effort. Although this difficulty may not be insurmountable within the present method, the approach may be changed altogether. It should be noted that this problem of particle superposition is inherent in the discrete element character of the method itself. Other hydrodynamic techniques treating the fluid as continuous should not be subject to this disadvantage.

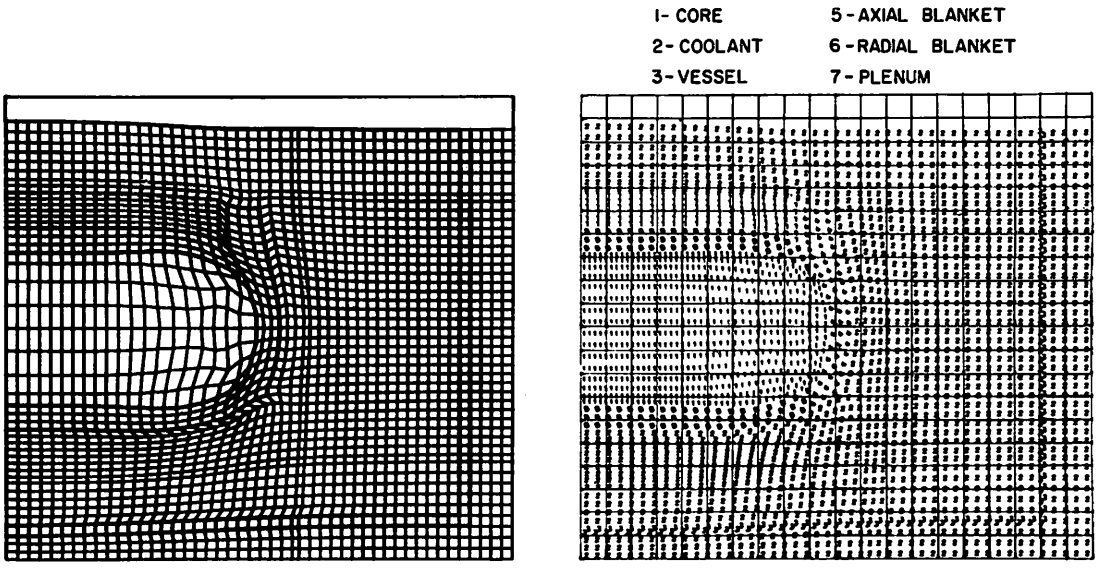
As apparent from the contents of this paper, the described Eulerian computer code and its adaptation to the fast reactor containment studies is still in its developmental stage. Therefore, the degree as to how much more this code will extend the study period of the excursion is still uncertain. The true extent of its application in the containment field has not as yet been fully determined.

In case the mentioned difficulties are satisfactorily resolved, attention will be directed in utilizing the advantages of a surrounding reactor vessel. The inclusion of a single reactor vessel into the code should not be a very major undertaking. The procedure in this design would be to use the prescribed pressure boundary condition to represent the reactor vessel.

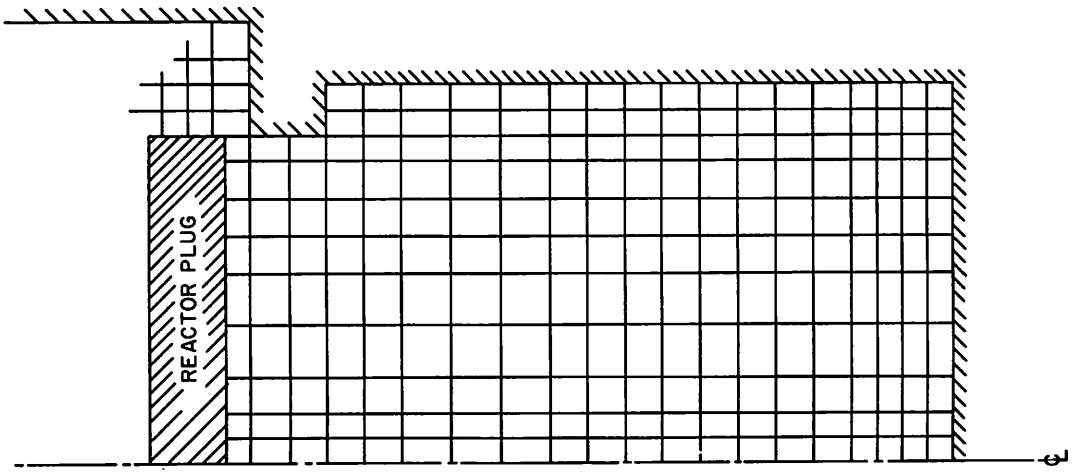
REFERENCES

[1] Chang, Y. W., Gvildys, J., Fistedis, S. H., "Two Dimensional Hydrodynamics Analysis for Primary Containment", ANL-7496 (November 1969).

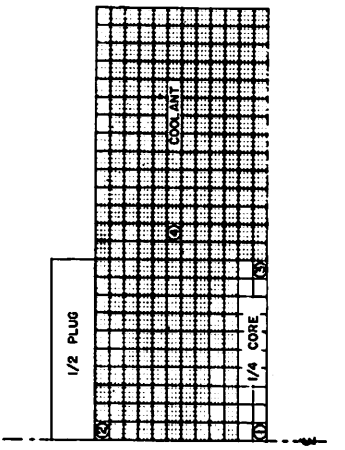
[2] Amsden, A. A., "The Particle-In-Cell Method for the Calculation of the Dynamics of Compressible Fluids", LA-3466 (February 1966).



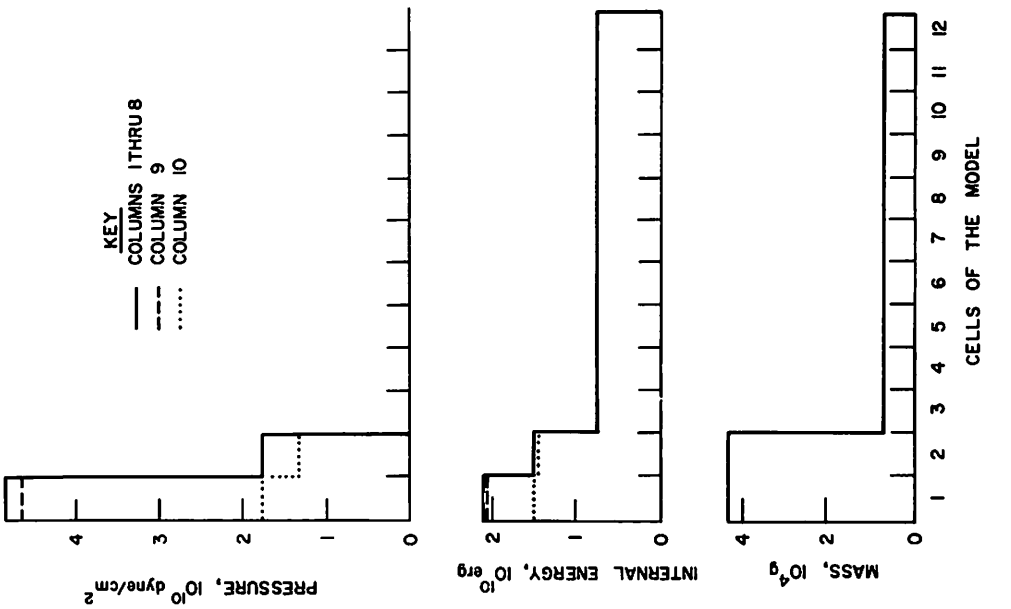
1. Sample Fluid Representation in Lagrangian and Eulerian Coordinates.



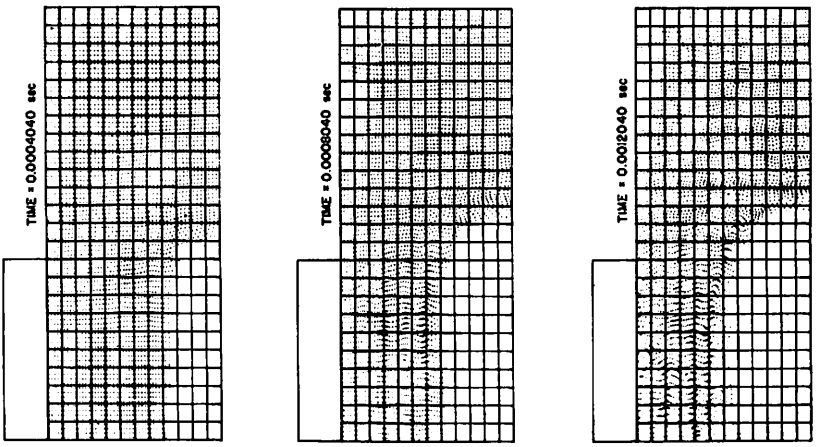
2. Computational Configuration of the Reactor Model.



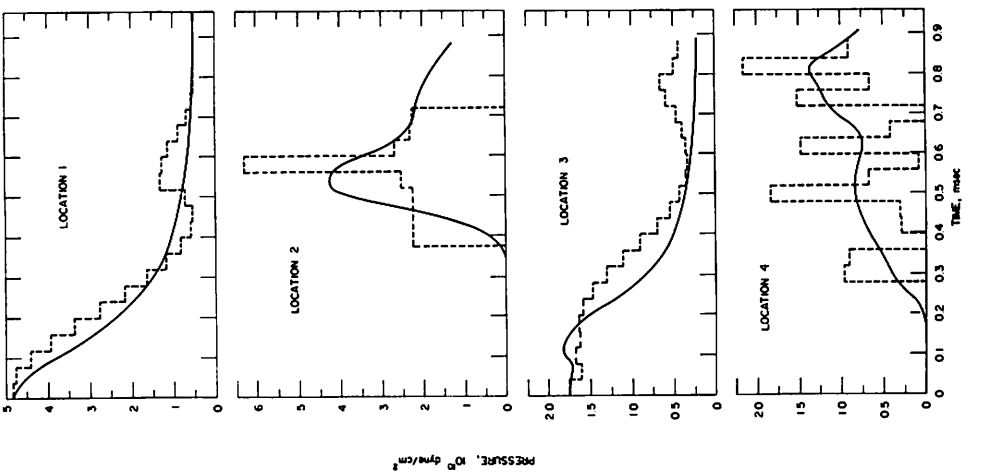
3. Initial Configuration of Sample Problem.



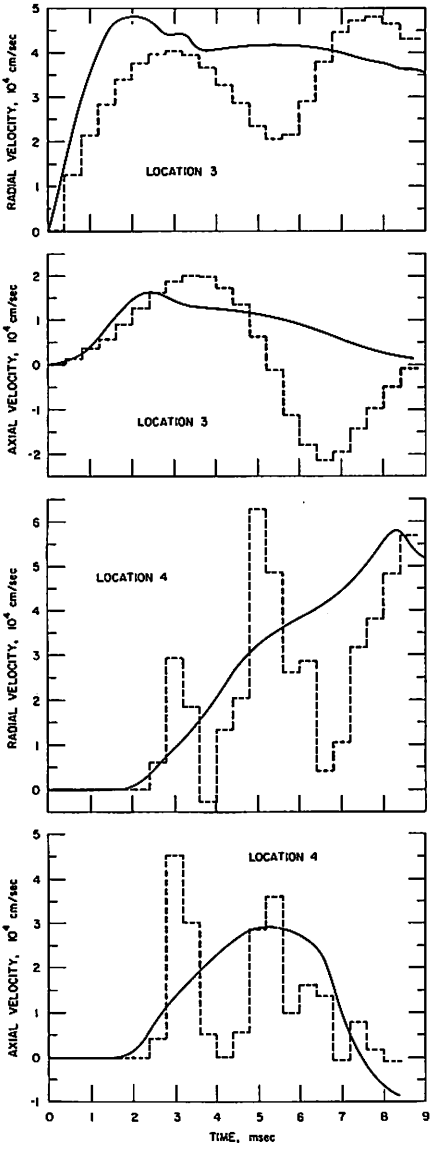
4. Initial Input Conditions of Sample Problem.



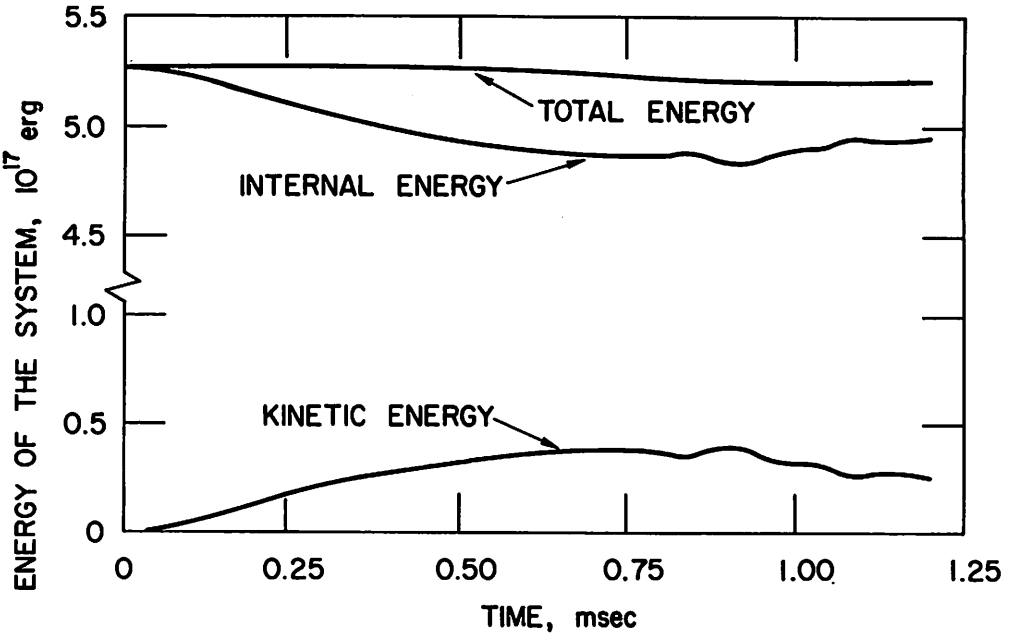
5. Typical Coolant Flow Configurations.



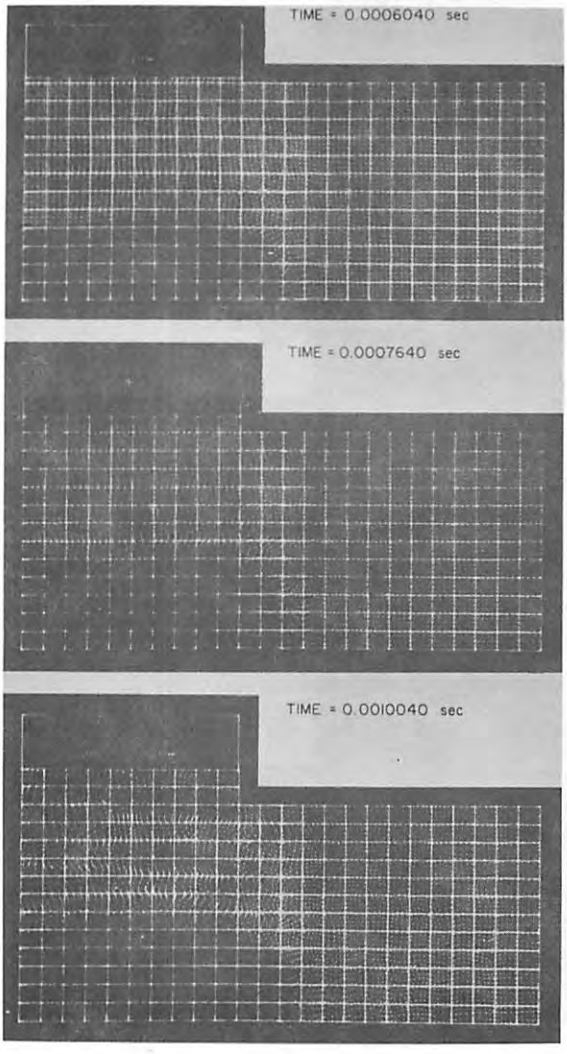
6. Pressure Histories at Different Locations.



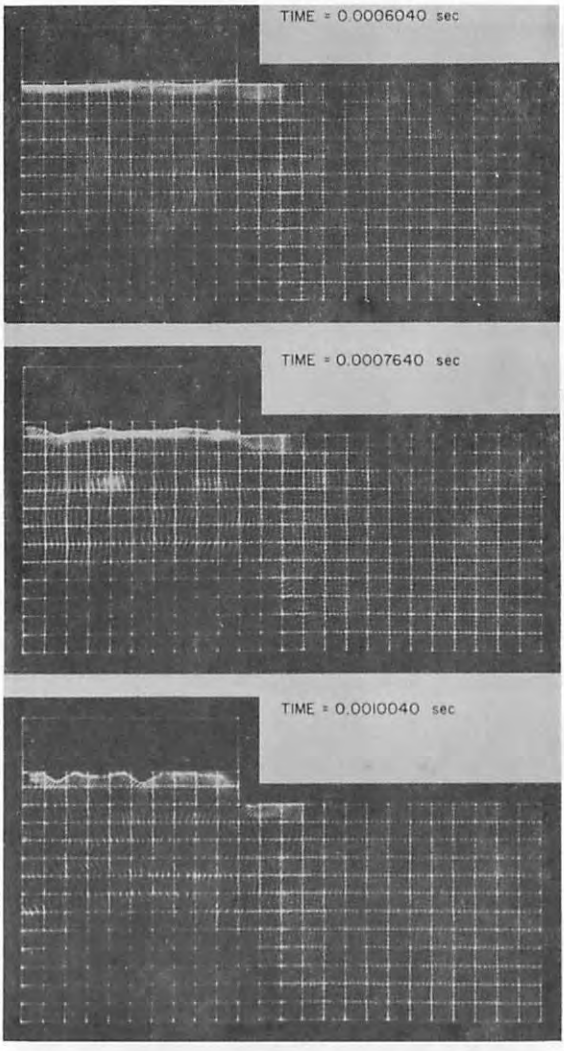
7. Velocity Histories at Locations 3 and 4.



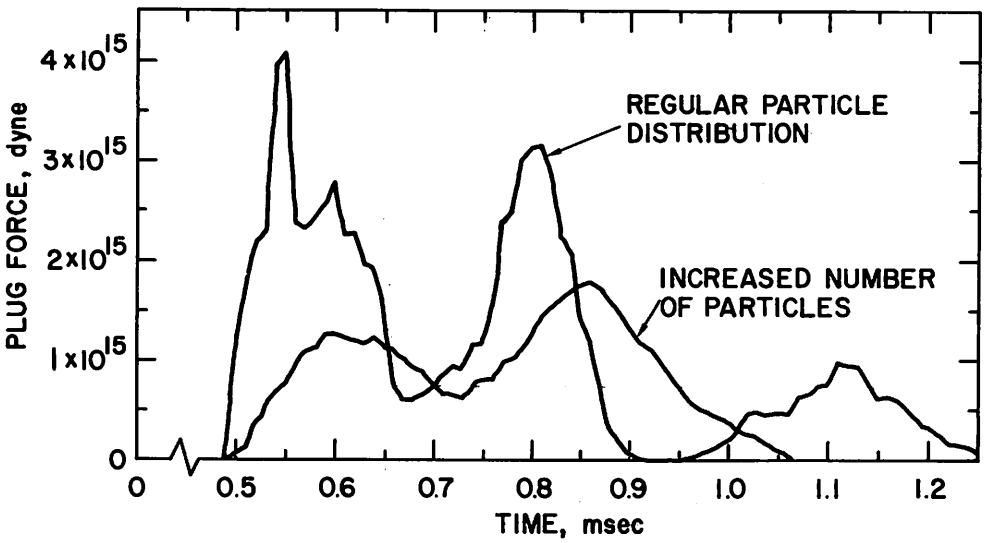
8. Energy Distribution of the Sample Problem.



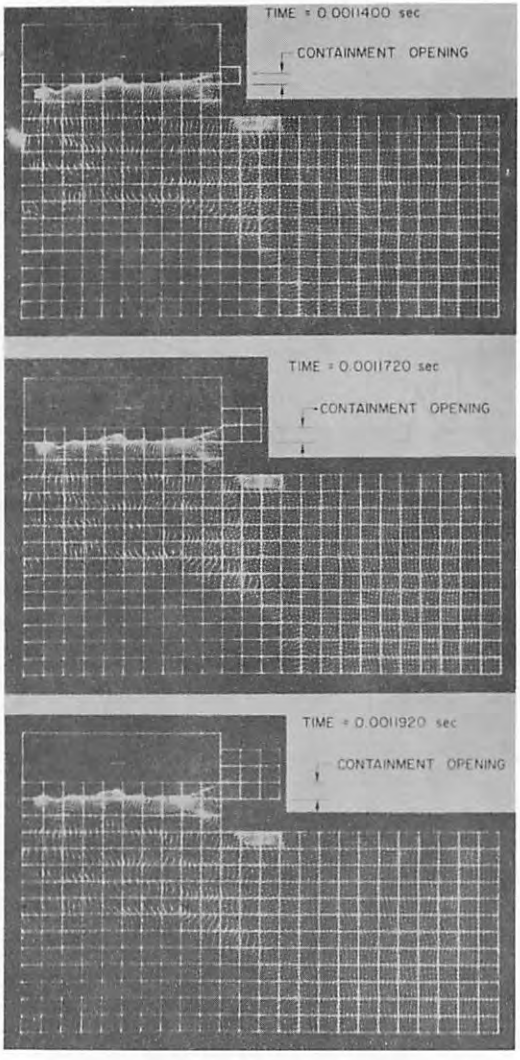
9. Relative Motion of the Plug with Respect to the Reactor.



10. Effect on Plug Movement due to an Increase in the Number of Fluid Particles.



11. Variation in Plug Force due to Different Number of Fluid Particles.



12. Display of Possible Coolant Spillage.