LA-UR - 74-243

TITLE: A PROPOSAL FOR COMPUTER INVESTIGATION
OF LMFBR CORE MELTDOWN ACCIDENTS

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SUBMITTED TO:

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RECEIVED BY TIC FEB 10 1976

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ABSTRACT

The environmental consequences of an LMFBR accident involving breach of containment are so severe that such accidents must not be allowed to happen. Present methods for analyzing hypothetical core disruptive accidents like a loss of flow with failure to scram cannot show conclusively that such accidents do not lead to a rupture of the pressure vessel. A major deficiency of present methods is their inability to follow large motions of a molten LMFBR core. Such motions may lead to a secondary supercritical configuration with a subsequent energy release that is sufficient to rupture the pressure vessel. The Los Alamos Scientific Laboratory proposes to develop a computer program for describing the dynamics of hypothetical accidents. This computer program will utilize implicit Eulerian fluid dynamics methods coupled with a time-dependent transport theory description of the neutronic behavior. This program will be capable of following core motions until a stable coolable configuration is reached. Survey calculations of reactor accidents with a variety of initiating events will be performed for reactors under current design to assess the safety of such reactors.

I. INTRODUCTION

Recent studies[1] have pointed out the severe consequences of a major accident involving the melting of the core of a liquid metal cooled fast breeder reactor (LMFBR) with subsequent breach of containment and release of large amounts of radioactive material to the environment. Plutonium is so toxic that the accidental release to the atmosphere of several hundreds of grams of this material would be a matter of serious concern. Because a typical LMFBR may contain as much as 1000 Kg or more of PuO_2, the release of as little as 0.01% of the available plutonium may be cause for alarm. It is hard to imagine an accident involving breach of primary and secondary containment that would not release this small percentage of the core materials to the environment. Indeed, it appears likely that substantially larger releases would occur. Also included in such releases following breach of containment would be large amounts of highly radioactive fission products. The probability of the occurrence of such accidents must therefore be shown to be almost zero.

In theory, the safety of fast breeder reactors can be established by either one of two approaches. First, we may seek to establish that the possibility of the melting of the core of such reactors is so exceedingly remote that such accidents need not be considered. Second, we may admit the possibility that such accidents can happen, however remote

the probability, and instead seek to guarantee that the melting of the core does not lead to breach of containment and release of radio-activity. In practice, a truly safe design will be obtained only if the probability of core meltdown and the probability of breach of containment following meltdown have both been minimized. Inattention to either of these areas may lead to an unsafe reactor concept.

Causes of hypothetical accidents involving the melting of the core of an LMFBR fall into several categories. Accidents such as the loss of flow with failure to scram and the overpower transient have already been examined in some detail. The physics of a core meltdown accident is complicated, involving neutron kinetics, fluid dynamics, heat transfer, and equations of state. Computational codes that have been developed to date can treat only the initial phase of a core meltdown accident, in which core material motions are small. Large scale motions of the molten core cannot be predicted by existing codes. It appears possible, however, that such large scale core movements can lead to a secondary supercritical configuration, with a subsequent energy release that may be larger than that of the original excursion. This secondary criticality is possibly a mechanism for rupturing the primary and secondary containments of an LMFBR system.

The Los Alamos Scientific Laboratory proposes to develop a calculational capability for describing the evolution of hypothetical accidents involving the melting of cores of fast breeder reactors with subsequent large scale motions of the molten core. These motions will be followed by means of implicit Eulerian fluid dynamics methods recently developed by group T-3 at the LASL. Two-dimensional, cylindrical geometry, time-dependent neutron transport methods will be used

to follow the neutronics excursions and to determine if and when a secondary critical configuration occurs. Group T-1 has considerable expertise in such calculations. Groups T-3 and T-4 at the LASL are expert in related fields such as heat transfer and equations of state.

A computer program will be written to implement this calculational capability. This program will be normalized as well as possible to existing data on reactor accidents and tests. Following normalization, a large number of reactor accidents with a variety of initiating events will be surveyed with this program to assess the likelihood of secondary criticality. Such surveys will be made for specific plants under current design. A major incentive for the development of such a computational capability is the relative low cost with which such surveys may be under-taken. Although a small number of experiments may ultimately be necessary to normalize the computational methods, an experimental survey comparable to the computational survey would be prohibitively expensive.

Section II.A of this proposal contains a brief discussion of ex-isting methods for describing core meltdown accidents. Several mech-anisms that can lead to a secondary criticality are presented in Sec. II.B. Section III contains a discussion of the methods we pro-pose to use to solve the secondary criticality problem. This section is divided into four subsections, which are devoted to the problems of fluid dynamics, neutronics, heat transfer, and equations of state, in that order. In Secs. IV - VI, we give a brief schedule for completion of the work proposed here, a list of the personnel to be involved with this project, and an estimate of costs.

II. BACKGROUND

A number of computer codes have been written for the analysis of hypothetical core disruptive accidents. These codes fall into three categories. Pre-disassembly codes like SAS-2A[2] are designed to predict phenomena occurring before the onset of a supercritical transient leading to core disruption. The output from a pre-disassembly code serves as input to a disassembly code, which follows core motions through this supercritical transient and predicts the total energy release. VENUS-II[3] is a typical disassembly code. Post-disassembly codes use the energy release and pressure histories predicted by a disassembly code to estimate reactor vessel damage.

A three stage approach is often used in reactor safety analysis. In a flow coastdown accident, for example, a pre-disassembly code is employed to predict the manner in which the initial sodium voiding, clad melting, and fuel slumping progress. The slumping of a partially melted core can lead to a supercritical core configuration. At this point, a disassembly code is used to follow the rapid neutron transient that may lead to substantial energy deposition and extensive core melting. Disassembly codes employ fluid dynamics methods to follow the resulting motions of the molten core. These motions quickly lead to a termination of the neutron transient, and the power level falls rapidly. The total energy released during this supercritical transient can then be calculated. An energy partition assumption or estimate is made, and post-disassembly codes are used to predict the final consequences of the accident.

Such a three-stage approach to reactor safety analysis overlooks a very real and important possibility. Tacit in the above analysis

is the assumption that, following disassembly, the core dissipates and generates no more energy. Because the core is at this stage largely molten and mobile, this assumption is not tenable without a thorough explanation of the mechanics of this core dissipation. It must be clearly demonstrated that it is unlikely that this molten core will ever reassemble in a supercritical configuration. In particular, large scale motions of the molten core must be followed to a stable coolable configuration.

Present reactor safety methods and codes are incapable of performing, and can not be modified to perform, this task. All current codes employ Lagrangian hydrodynamics methods, which are unsuited for the prediction of large core motions. All these codes fail when material motions greater than several centimeters occur. A brief discussion of existing methods is given in Sec. II.A. below.

We propose to develop an integrated computational package for disassembly analysis that can follow large scale motions of a molten core until a stable configuration is reached. The possibility of a secondary critical configuration will be examined. This code package is intended to supplement, not replace, the existing pre- and post-disassembly codes. It will, however, provide a more accurate and much more extensive description of the disassembly process.

There are several postulated chains of events that may lead to a secondary critical configuration for a molten core. The initial disassembly can eject a molten slug of fuel upwards into the fission gas plenum. This slug can then fall back into the core region to give a critical configuration. If this slug fails to re-enter the core, the remainder of the core can pool on top of the lower axial shield, yielding a critical configuration (a puddle of 40% of the total fuel is critical). Several of these mechanisms for arriving

at a secondary critical configuration are discussed further in Sec. II.B.

A.   Existing Methods

Several numerical tools are currently available to study LMFBR core meltdown phenomena. The SAS-2A code, now operational on the LASL CDC 7600 computer, utilizes a multi-channel approach to predict sodium boiling and voiding dynamics for flow coastdown or power/flow mismatch accidents. The LASL version of the code predicts fuel, cladding, and sodium temperatures as functions of time. Clad dryout (sodium film evaporation) is also explicitly calculated. The code will predict core material temperatures and the sodim voiding profile prior to slumping. SAS-2A is a pre-disassembly code designed to calculate all phenomena occurring before fuel slumping and subsequent core meltdown. Similar calculations are performed by the FREADM[4] code developed at General Electric (GE), Sunnyvale, and the MELT-II[5] code developed at Hanford Engineering Development Laboratory (HEDL).

The slumping of a partially melted core may lead to a prompt critical core configuration and may give rise to reactivity insertion rates in the range $0 to $50/sec. Numerical methods[6] are currently being developed by Argonne National Laboratory (ANL) to operate in conjunction with SAS to predict these reactivity insertion rates

The state of the reactor at its prompt critical configuration calculated by SAS is input to the VENUS-II[3] disassembly code. VENUS-II predicts the energy deposition in the core material due to the prompt critical neutronics excursion. VENUS-II is a two-dimensional coupled neutronics-hydrodynamics code. Lagrangian hydrodynamics is used and the neutronics is performed with point kinetics and a perturbation theory treatment of reactivity feedback due to material motion. While other disassembly codes exist, VENUS-II has been widely accepted

and used throughout the country. Other examples of disassembly codes are MARS[7] and PAD.[8]

A more accurate neutronics calculation will be performed by the FX-2[9] code. FX-2, like VENUS-II, is a disassembly code that utilizes two-dimensional Lagrangian fluid dynamics. The neutronics, however, is treated in a quasistatic diffusion theory fashion. The basis for this approach lies in the QX-1[10] space-time fast reactor kinetics code. FX-2 is still in a developmental stage.

Accurate neutronics calculation in disassembly analysis is not a new concept. Transport theory neutronics was used in the one-dimensional (spherical geometry) AX-1[11] code in 1959 and again in 1968 with the FRAP[12] code of Atomics International (AI). FRAP, a more sophisticated version of AX-1, included Doppler feedback and a more elaborate equation of state. A simple study[13] of secondary criticality was performed with FRAP, but few general conclusions could be drawn.

The objective of both VENUS-II and FX-2 and indeed the objective of all present disassembly codes is to predict the energy deposition during a prompt critical fast reactor excursion. Both codes are limited to computing the very small material motions (a few centimeters) that occur during the excursion. This limitation is due to the Lagrangian formulation of the fluid dynamics equations.

The reactor primary vessel may be damaged due to an accident in one of several ways. Fuel vapor pressure may do PdV work on the vessel by virtue of its expansion. In mild prompt critical bursts in which disassembly pressures are low, the vessel integrity is not threatened by this mechanism. Even in a mild excursion, however, large portions of the core are melted and ejected toward the surrounding sodium. In

this case, a large fuel coolant interaction may take place in which the pressures generated act to lift a slug of sodium toward the vessel head, threatening vessel integrity. Several codes are currently in use to treat this fuel-coolant interaction. The "ANL parametric model"[14] has several variations, and a new formulation is currently being developed.[15] (Most of the variations are reported in limited distribution reports and cannot be cited. One variation is reported in Ref. 16.) An analogous code, SOCOOL[17] was developed at HEDL. The SAS/FCI model,[18] developed at ANL, is a fuel-coolant interaction method used in conjunction with an unreleased version of SAS to calculate accident phenomenology for the unprotected overpower transient accident. MELT-III,[19] a developmental code at HEDL, also computes fuel-coolant interaction phenomena for the overpower transient case.

Once fuel has been dispersed out of the core region, the vessel may be further damaged by melting as a result of decay heat generation. Few numerical methods are in widespread use to treat this post accident heat removal problem. Uncertainties in material configurations and heat transfer mechanisms obviate the need for sophisticated computer programs at this time. An important contribution of our method, however, will be an explicit prediction of the position of core materials following disassembly. This prediction will allow a more precise treatment of the post accident heat removal problem, precluding the need for excessively pessimistic assumptions. The amount of fuel leaving the upper plenum region will be explicitly predicted, as well as the amount of fuel remaining in the core region following all secondary excursions.

The final aspect of accident analysis lies in the prediction of reactor vessel stress and strain due to forces created in the disassembly stage of the accident. Several versions of the REXCO code, developed

at ANL, are used to analyze vessel response. Examples are REXCO-H (Hydrodynamic), REXCO-HEP (Hydrodynamic-Elastic-Plastic), REXCO-HT (Heat Transfer), REXCO-IL (Inelastic-Lagrangian), and NASTRAN.[20-22] At GE the RECORD code is used to study vessel response. All of these codes accept pressure histories as input. The propagation of these pressures is then calculated explicitly, and dynamic stress and strain equations are applied to the reactor vessel and components. A disassembly or fuel-coolant interaction code usually supplies this pressure-time curve.

B. Secondary Criticality

There is no currently available tool for evaluating the likelihood and consequences of secondary criticality in LMFBR accidents. The methods discussed in the above section can be used only for predicting the initial core meltdown phenomena. Following meltdown, large-scale motions of the core are inevitable. Such large-scale core motions can lead to a second supercritical configuration. Several mechanisms by which the core can reassemble in a critical configuration are discussed below for one kind of hypothetical core disruptive accident. Other kinds of accidents involve similar phenomena.

Figure 1 is a schematic representation of a typical LMFBR core and externals. This figure depicts only the reactor components which are of interest in recriticality studies. In Figs. 1 and 2, fuel is indicated by criss-cross hatching, liquid sodium is represented by stippling, and relocated steel is indicated by horizontal hatching. This particular reactor has massive radial and lower axial neutron shields. These shields contain the core in a massive bucket. Molten core materials can not escape appreciably in a radial or downward direction.

Consider, as an example, an accident involving a loss of flow without scram. In the predisassembly portion of the accident, SAS-2A may be used to predict sodium boiling and voiding from the core region with commensurate clad and fuel heating and melting. SAS often predicts[23] that the sodium is expelled from the core and fission gas plenum except for the outermost ring of fuel. Some steel melts and is presumed[*] to run down into the lower axial shield, plugging the subassemblies

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[*]The relocation and freezing of steel remains a crucial question in recriticality analysis. The steel, once frozen, tends to plug up sub-assemblies and inhibit core cooling as well as to inhibit the downward escape of fuel material. Work is in progress at ANL to study this plugging effect.
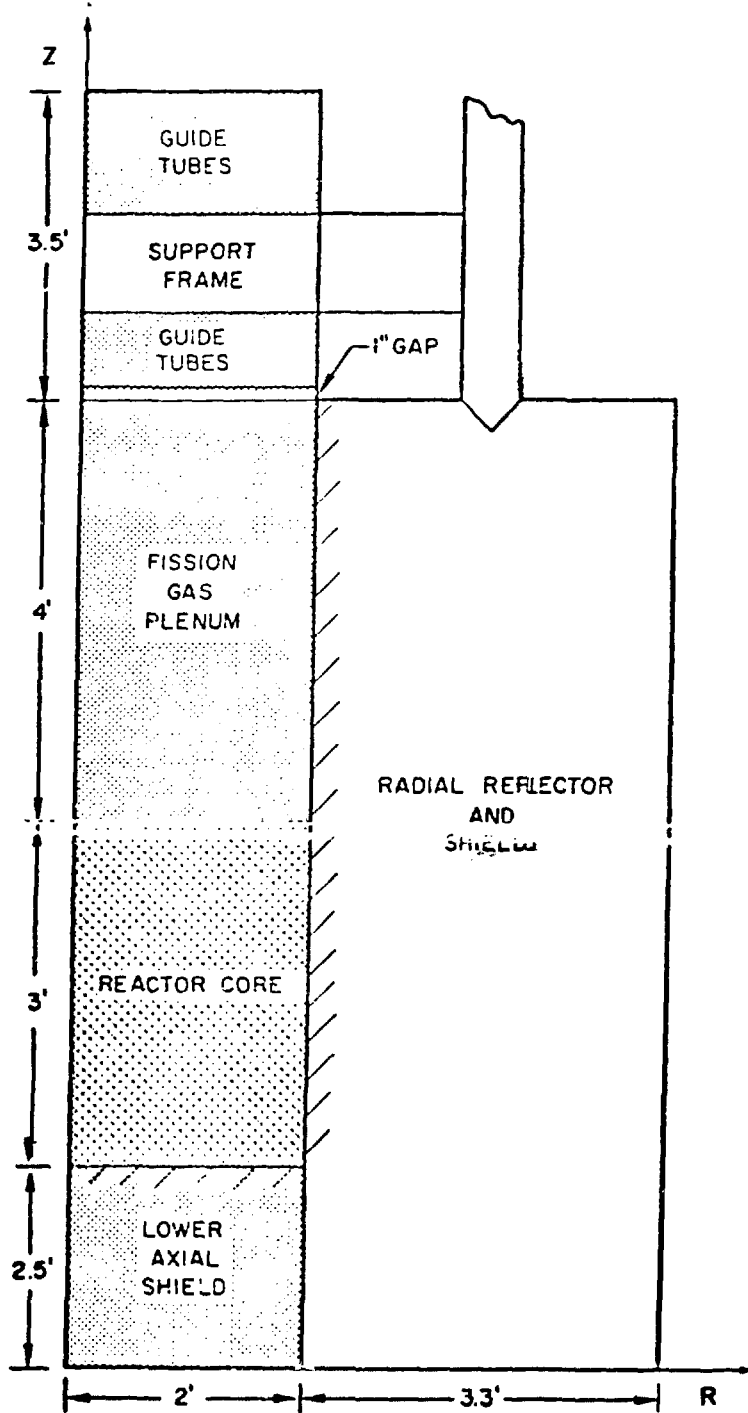
Figure 1

Typical LMFBR Core at Steady State.

to some extent. The fuel in the central region of the reactor now melts and slumps, with the pin stubs above the molten region falling down. A perturbation theory analysis indicates that the reactor is, at this point, prompt critical due to fuel slumping and is experiencing about a $20/sec reactivity insertion.

During the prompt critical neutronics excursion, a large amount of energy is deposited in the core. Most of the core melts, and modest vapor pressures (10's of atmospheres) which develop in the core center disperse some of the central fuel. The motion may be predominantly in an axial direction, since subassembly can walls may retain some of their strength at this stage of the accident. Fuel in outer core regions remains essentially stationary, because the time elapsed since prompt criticality is insufficient for appreciable motion due to gravity. The fuel being ejected axially is at an average temperature of around 4000°K and attains a velocity of approximately 1000 cm/sec. The fuel moving downward may have its motion impeded or stopped by the relocated steel which has plugged the lower axial reflector.

Ensuing events are crucial in determining the probability of occurrence and the severity of a secondary criticality. Our present lack of understanding of the material dynamics from this point on preclude definitive conclusions. For example, consider the trajectory of the upper slug of fuel being ejected from the core. Three possibilities exist for the motion of this slug:

(1) It may flow unimpeded through the fission gas plenum and out the top of the guide tubes.

(2) It may melt steel as it attempts to pass through the plenum, cooling itself below the heat of fusion of UO_2, and freeze in place. Alternately, it may crush plenum tubes ahead of it, in a "log jam" fashion, once again being brought to rest.

(3) It may interact with some portion of the sodium above the

core and generate pressures which may blast some of the fuel

back down into the core.

In possibility (2) the fuel may fall or drop back down into the core.

Unless cooling is sufficient, decay heat will melt whatever fuel has

solidified, allowing it to drop back into the core as well. Reentry

of the ejected fuel material is one mechanism for recriticality in this

accident. Another mechanism for recriticality is the collapse of the'

molten fuel which has remained in the core during or after the axial

ejection of the slug.

The core material dynamics is, in all likelihood, a combination

of all of the phenomena mentioned above. The exact sequence of events

is impossible to predict without a coupled modeling of the important

phenomena which interact in the problem. Current recriticality studies

utilize crude estimates of the thermal and hydraulic behavior of core

materials following VENUS-II calculations. All methods presently in

use are inaccurate. To evaluate the potential hazard from recriticality,

the coupling in an integrated package of all of the various involved

processes is imperative.

Accurate treatment of the time dependent neutronics is equally

important. A point kinetics or a quasistatic diffusion theory approach

to the secondary criticality neutronics problem is insufficient. The

extensive material motions in the recriticality problem automatically

preclude the use of point kinetics. (The assumption of a constant

spatial flux distribution is clearly incorrect.) Diffusion theory is

likely to be inadequate. Regions which are almost completely voided

of material will occur. These regions give rise to very large diffusion

coefficients, which slow convergence of iterative methods for solving
the finite difference approximation to the diffusion equation. Even
when the problem is soluble using diffusion theory, the result will be
incorrect in a nonconservative fashion; that is, diffusion theory will
usually underpredict multiplication. For example, calculations were
performed using the 2DB (diffusion theory) portion of DOT-2DB[24] and
TWOTRAN-II[25] on a configuration similar to that shown in Fig. 2. In
our model, only the outermost ring of fuel remains standing. A portion
of the remaining fuel is puddled on top of the steel plug formed in
the lower axial reflector, while a large slug of molten fuel is assumed
to move toward it from above. Figure 3 shows a plot of k_{eff} versus
slug-puddle separation S for diffusion and transport theory. Diffusion
theory predicts that the reactor is at no time prompt critical.[*] TWOTRAN
predicts that the system is prompt critical at a slug separation of
around 5cm and that the excess reactivity as S approaches 0 is around
$9. More than enough excess reactivity is available in this system
to allow a sizable secondary excursion which diffusion theory would
not have predicted. Hence, the use of transport theory is necessary
in the study of secondary criticality.

While the reactor design shown in Figs. 1 and 2 is a specific one,
other designs are likely to present similar features and potential for
recriticality. The problem of fuel recompaction following core melt-
down and disassembly is a general problem, indigenous to fast, high
power density reactors. Whenever coolant passages are blocked for any

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[*]The ordinate in Fig. 3 is normalized to a reference reactor calculation
in which K_{eff} = 1.0176. Since β_{eff} = 0.03157, prompt criticality occurs
at K_{eff} = 1.021.
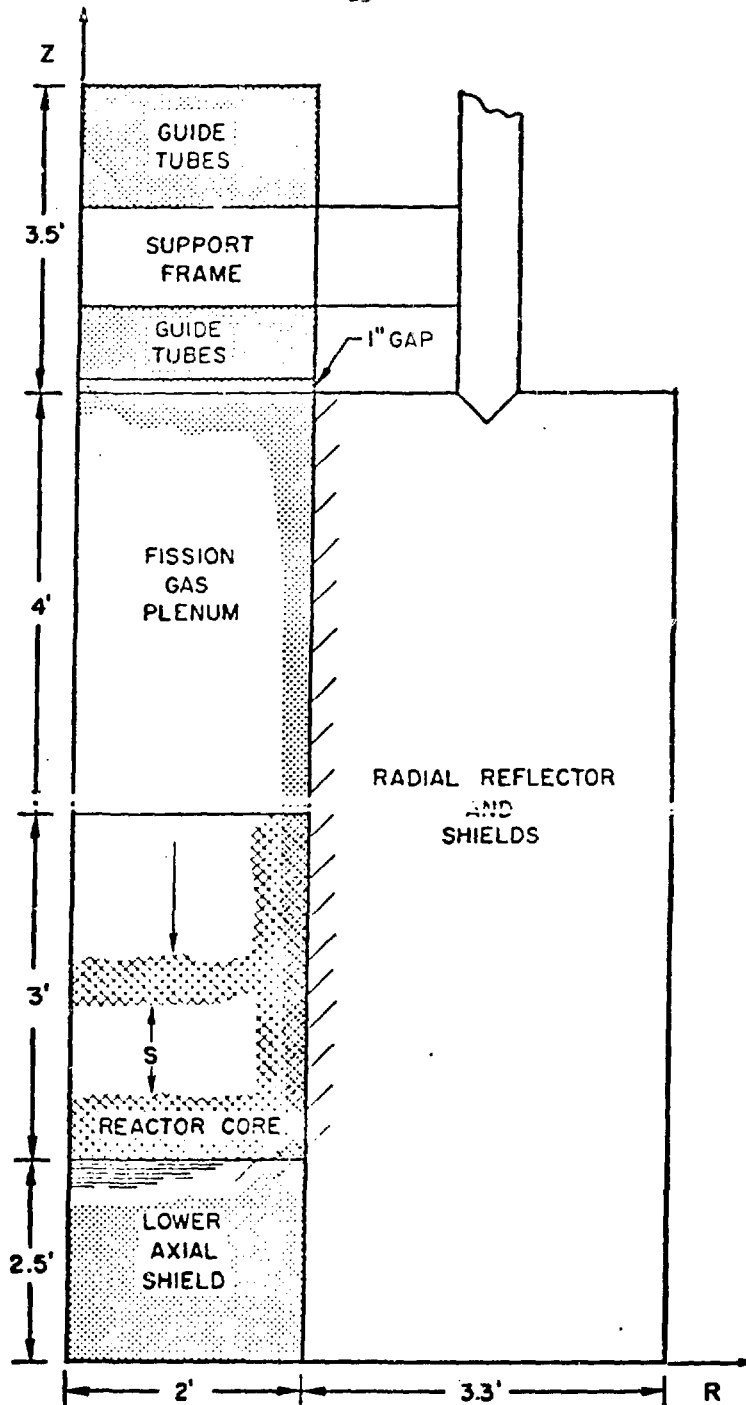
Figure 2

Postulated Core Recompaction for Diffusion vs.
Transport Theory Comparison.
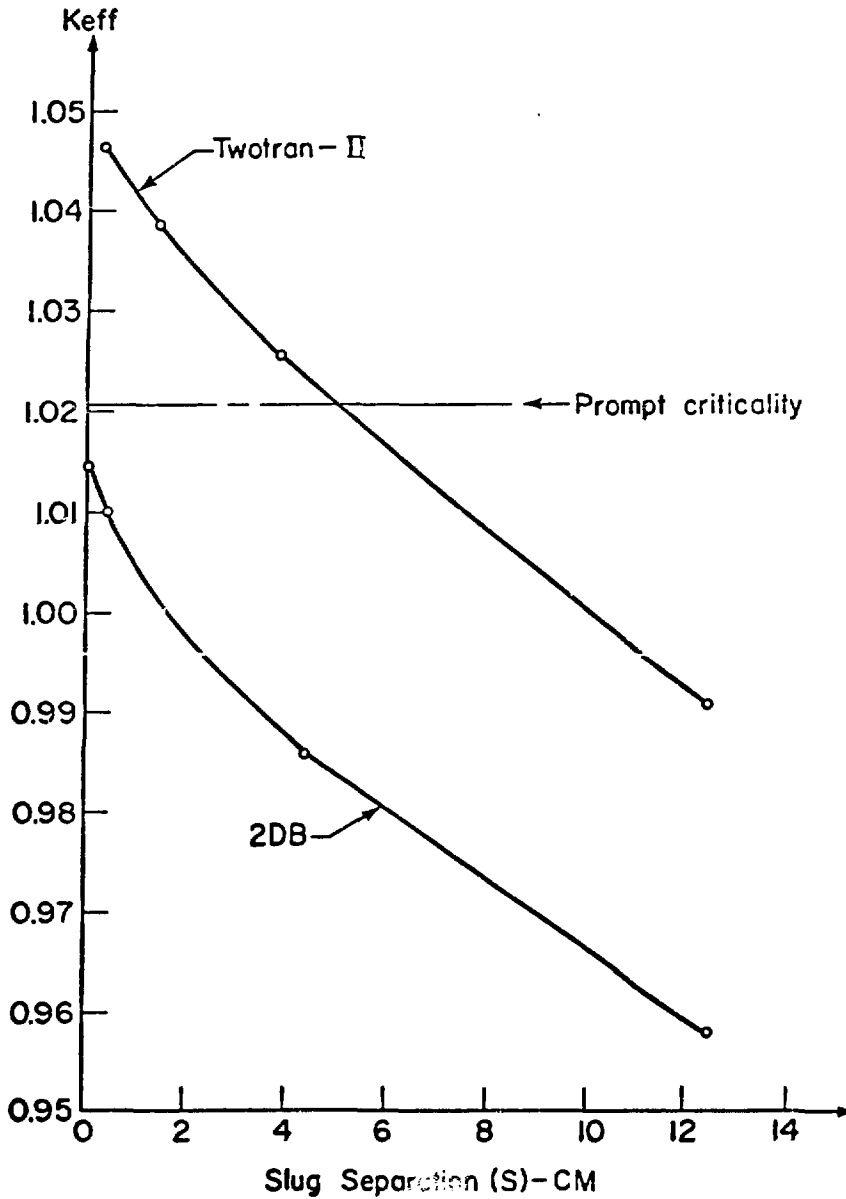
Figure 3

Diffusion Theory vs. Transport Theory for a Slug
Recompaction Recriticality Calculation.

appreciable amount of time, the potential exists for sodium boiling,

voiding, and eventual melting of fuel. This process may also occur

in the overpower transient accident if coolant channels become blocked

with debris ejected after the transient. If melting and slumping of

some part of the core leads to a mild prompt critical burst which melts

the majority of the core, but does not permanently disperse the fuel,

then the stage is set for recriticality.

III. PROPOSED METHODS

The physics of a core-meltdown accident is complicated, involving the coupling of neutronic processes that generate a large amount of heat with mechanical and thermodynamical processes that dissipate this heat in a variety of ways. Methods for following the evolution of such an accident fall into four categories: fluid dynamics, neutronics, heat transfer, and equations of state. We discuss particular methods from each of these categories in the following four sections of this proposal. These methods will adequately treat the more important aspects of the secondary criticality problem.

The coupling of methods from each of the above four categories into a single algorithm is not difficult. We have proposed methods that make this coupling as simple as possible. The use of a fixed Eulerian grid throughout the course of the calculation by both fluid dynamics and neutronics methods leads to a major simplification. In particular, cross sections necessary to the neutronics calculation can be generated easily from the densities output from the fluid dynamics calculation. Energy production rates generated by the neutronics calculation can be input directly to the fluid dynamics algorithms.

We expect a typical calculation to proceed in the following manner. A core configuration computed by SAS serves as an initial condition for our computer package. We assume for the present discussion that this core configuration is supercritical. During the ensuing neutron transient, a relatively large number of neutronics time steps with small time step sizes are taken. Fluid dynamics time steps are interspersed with the neutronics steps. During this initial phase of the accident the emphasis is on the neutronic behavior of the reactor because material velocities are small but neutron flux changes are large. When material motions have terminated the neutronics excursion and the power

level has fallen to a suitably low level, the neutronics time step
is lengthened. Conversely, since material velocities are now large,
fluid dynamics time steps may be decreased. During the next stage of
the accident, the neutronics calculation serves mainly as a check on
the subcriticality of the system. Therefore, the neutron flux must be
updated only after appreciable material motion. If a configuration is
reached in which the power level begins to rise, then neutronics time
steps are shortened in preparation for a possible secondary excursion.
This secondary excursion is treated with neutronics and fluid dynamics
time steps appropriate to flux changes and material velocities occur-
ring at this time.

A number of auxiliary computations may be performed periodically
during the course of the above computation. Estimates of heat transfer
during the relatively long times involved here may be necessary. Regen-
eration of neutron cross section sets will probably be needed at
certain times. Movement of delayed neutron precursors must be considered.
Such auxiliary phenomena are considered in the appropriate sections below.

A. Fluid Dynamics

Numerical fluid dynamics calculations is a field of effort in which
the LASL has excelled for three decades. For a large variety of scien-
tific and engineering purposes, this laboratory has developed a succes-
sion of new and powerful computer methods and has applied these with
consistent success to investigations in virtually every branch of mod-
ern technology, from problems in weapons design and effects analysis
to the study of tornadoes and the extraction of geothermal energy.
The center for this activity is Group T-3 of the Theoretical Division,[26]
which is the group that will maintain specific responsibility for the
fluid dynamics work described in this proposal. In this section, we

present a brief outline of the techniques that will be employed in this aspect of the investigation.

To calculate the dynamics of materials in the LMFBR during a molten-core accident is impossible in complete detail, because of the complex mixtures of material kinds and states. The solid and liquid parts consist of chunks or droplets of various sizes, interacting with each other and with the vapors of sodium and fuel. Our basic assumption, however, is that the features of interest do not depend on the exact details of structure, but only on some lowest-order moments of the complex configuration. The situation is analogous to that of molecular dynamics, in which the behavior of every molecule is neither possible to calculate nor necessary to know for most purposes, such low order moments as density, pressure, and velocity being sufficient.

Even with the assumption that the fine-scale structural details can be ignored, the mathematical formulation and numerical solution are both quite complicated in their most general form. Accordingly, we have looked for a model that is both relatively simple in its initial stages of development, but also easily capable of generalization as the investigation progresses.

The essence of this model can be described in terms of two inter-penetrating substances, "fuel" and "vapor". The former is visual-ized to be globules of liquid or solid fuel, together with fragments or components of other materials such as steel. The latter is com-posed of the vapors of sodium, fuel, and perhaps of other materials. In our initial model, we assume that the fuel globules are homogeneous in their composition, each of the same size and consisting of the same proportionate mixture of actual fuel, steel, and perhaps other materials. The vapor, however, is not appropriately treated as homogeneous; we

assume that its principal constituents are fuel and sodium, in proportions that vary with position and time as a result of phase transitions in the fuel and diffusion between vapors, but not as a result of different local convective velocities. It is also assumed that local pressure equilibrium is maintained between each globule and the vapor surrounding it, which is equivalent to assuming that sound signals can traverse the scale of a globule in a time short compared with the time for appreciable local velocity changes.

A primary variable in the analysis is θ, the local fraction of volume occupied by the vapor. Correspondingly, $1-\theta$ is the local fraction of volume occupied by the fluid. Thus, θ corresponds to the porosity function in the theory of fluid motion through porous media. Analogous to the permeability, it is necessary to describe in our model the relative mobility of the vapor relative to the fuel. When the fuel globules are closely spaced, the vapor is trapped and can maintain a high degree of compression (and pressure) for sufficient time to accelerate the fuel strongly. When the fuel globules are dispersed, the relative mobility is great; the vapor can rush past the globules (or vice versa) with only the relatively mild interaction induced by drag.

Pressure is assumed to develop only by virtue of vapor heating and/or compression. Validity of this assumption requires the fuel globules to be essentially incompressible, and never to be completely free of interspersed vapor. Accordingly, we require an equation of state for the vapor, which sums the partial pressures for the two components

$$p = f_1(\rho_1, I_1) + f_2(\rho_2, I_2) \quad,$$

in which ρ is density, I is specific internal energy, and p is the pressure.

For our purposes, two types of density are convenient. One of

these, without a prime, denotes the actual microscopic density of the material; the other, with a prime, denotes the mass of material per unit total volume. With subscripts v and f for vapor and fuel, respectively, we can thus write

$$\rho'_v \equiv \theta \, \rho_v \quad , \tag{1}$$

$$\rho'_f \equiv (1-\theta) \, \rho_f \quad . \tag{2}$$

We note that θ denotes not only the volume of vapor per unit total volume, but also the cross-sectional area of vapor per unit total cross section, for which the scalar nature of θ indicates that we have assumed isotropy. Invoking this dual nature for θ and examining carefully the balance of mass fluxes into and out of a control volume, one can show that the appropriate equations for mass conservation are

$$\frac{\partial \rho'_f}{\partial t} = - \nabla \cdot (\rho'_f \, \vec{u}_f) - S \quad , \tag{3}$$

$$\frac{\partial \rho'_v}{\partial t} = \nabla \cdot (\rho'_v \, \vec{u}_v) + S \quad . \tag{4}$$

in which $\vec{u}_f$ and $\vec{u}_v$ are the velocities of fuel and vapor, respectively, and S is the rate of fuel mass vaporization per unit volume. Alternatively, these two equations can be written

$$\frac{\partial \rho_f (1-\theta)}{\partial t} = - \nabla \cdot \left[\rho_f (1-\theta) \, \vec{u}_f \right] - S \quad , \tag{5}$$

$$\frac{\partial \rho_v \theta}{\partial t} = - \nabla \cdot \left(\rho_v \, \theta \, \vec{u}_v \right) + S \quad . \tag{6}$$

With ρ_f identically constant (the incompressibility assumption for fuel globules), Eq. (5) becomes

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left[(1-\theta) \; \vec{u}_f \right] - S/\rho_f \quad . \tag{7}$$

from which the variations of θ can be determined if S and $\vec{u}_f$ are known.

For most dynamical purposes, it is not necessary to examine the subdivision of ρ_v into ρ_1 and ρ_2, the partial densities of the fuel and sodium vapors. But to the extent that this may be required for the equation of state, or any other purpose, we may write

$$\frac{\partial \rho_1'}{\partial t} + \nabla \cdot (\rho_1' \; \vec{u}_v) = S + D$$

$$\frac{\partial \rho_2'}{\partial t} + \nabla \cdot (\rho_2' \; \vec{u}_v) = - D$$

in which D describes the relative diffusion.

We also can examine the balance among fluxes and exchanges of momentum, resulting in the following dynamical equations:

$$\rho_f' \left[\frac{\partial \vec{u}_f}{\partial t} + (\vec{u}_f \cdot \nabla) \vec{u}_f \right] = - \nabla[p(1-\theta)] + \nabla \cdot \; \mu_f (1-\theta) \nabla \vec{u}_f$$
$$+ K(\vec{u}_v - \vec{u}_f) + \rho_f' \; \vec{g} \quad , \tag{8}$$

and

$$\rho_v' \left[\frac{\partial \vec{u}_v}{\partial t} + (\vec{u}_v \cdot \nabla) \vec{u}_v \right] = - \nabla(p\theta) + \nabla \cdot (\mu_v \theta \nabla) \vec{u}_v$$
$$+ K(\vec{u}_f - \vec{u}_v) + \rho_v' \; \vec{g} \quad . \tag{9}$$

The two viscous terms, with coefficients μ_f and μ_v, have here been expressed in highly simplified fashion, their purpose being only to remove negative diffusive truncation error effects from the numerical solutions in the manner of a generalized artificial viscosity. K is a

function describing the exchange of momentum between fuel globules and vapor. The dependence of K on θ must express the loss of vapor mobility as the fuel globules come together; the dependence on $|\vec{u}_f - \vec{u}_v|$ describes the drag, which combines both viscous and flow-separation effects. The gravitational acceleration is denoted by $\vec{g}$; its inclusion is probably of significance only for the fluid-globule dynamics.

The third step in deriving the required equations comes from an examination of energy variations. Assuming local thermodynamic equilibrium in the vapor assures that a single temperature function is sufficient to describe both fuel vapor and sodium vapor at each time and place. Combining the various contributions to the energy equations, we may derive the following

$$\rho_f'\left[\frac{\partial I_f}{\partial t} + (\vec{u}_f \cdot \nabla) I_f\right] = E + R(T_v - T_f) - E_v + \nabla \cdot [k_f(1-\theta)\nabla T_f] \quad , \quad (10)$$

$$\rho_v'\left[\frac{\partial I_v}{\partial t} + (\vec{u}_v \cdot \nabla) I_v\right] = R(T_f - T_v) + K(\vec{u}_f - \vec{u}_v)^2 - p\nabla \cdot [\theta\vec{u}_v + (1-\theta)\vec{u}_f]$$

$$+ \nabla \cdot k_v \theta \nabla T_v + E_c \quad . \quad (11)$$

E_v and E_c represent heat absorption or release rates from vaporization or condensation, E is the rate of energy production in the fuel from nuclear reactions, R is an exchange coefficient for the transfer of heat from fuel globules to vapor, and k is a conduction coefficient for heat. Heat conduction in the fuel is represented by the coefficient k_f, which will have to depend on θ in such a way as to vanish when the fuel globules are so sparse as to be isolated from each other. Likewise, k_v should vanish as θ becomes small and the vapor pockets become disconnected. It should be noted that for R small, isolated fuel globules may remain almost constant in temperature. The K term in Eq. (11) expresses the dissipation from drag effects, which is assigned entirely

to the vapor; viscous dissipation is probably negligible, but can be
easily inserted if necessary. Work terms from the fuel globule motion
are assigned to heating the vapor, since it is solely the potential
energy of the vapor that contributes to this process.

Several of the functions symbolized in this discussion have not
yet been specified here, notably the equations of state, the drag
function, K, the energy production and coupling functions, the phase
transition rates and corresponding latent heat exchange, and the
relations between specific internal energy and temperature. Apart
from these, the number of unknown field variables is the same as the
number of equations. The drag function, K, however, may appropriately
introduce another field variable, r, the mean linear dimension of a
globule, which can vary with position and time. A constant value for
r will serve as a useful first approximation, from which we can derive
information concerning the dependence of the results on the choice of
globule scale. An improved version of the study will represent more
realistically the processes of globule rupture and coalescence by means
of a transport equation for r. The energy production rate from nuclear
reactions is another important function for which accurate determina-
tion requires extensive calculations, in this case furnished by the neu-
tronics techniques discussed elsewhere in this document. The discussion
has so far omitted a consideration of the flow interaction with structural
elements, which may be significantly non-isotropic in orientation. To
incorporate these effects will require interaction terms representing the
added inertia, the non-isotropic drag, and the dissipation of energy.
Yet another potentially significant feature that we expect to incorporate
into the analysis is the explosive liquid-liquid interaction that can occur

when liquid fuel globules come into contact with liquid sodium, which may be waiting in the peripheral regions. If such interactions occur, the resulting violent pressure pulse can alter the dynamics in ways that may possibly mitigate the chance of secondary criticality.

The calculation of specific examples by means of the equations derived in this section will require the specification of realistic initial and boundary conditions. Some consideration of this matter has been required by the investigators who have utilized the VENUS-II code to examine the early stages of disassembly. In the present case, however, the calculations will cover a considerably larger domain and extend through a considerably greater period of time. Part of the uncertainty of the results will be related to the questionable nature of both the initial state and boundary conditions. As emphasized elsewhere, however, our goal is to show the dynamics that can be expected from all reasonable variations of both the prescribed conditions and the material properties. If these studies can demonstrate that secondary criticality is not possible for such a range of variations, then they will serve as a solid basis for refuting claims of possible disaster from the LMFBR. Even though we may not know exactly which calculation might correspond to an actual set of accidental circumstances, an analysis of the full spectrum of possible cases will lend considerable confidence to our conclusions.

The numerical methods to be used in accomplishing these calculations will be assembled from several computer techniques that have already been developed by Group T-3. The experience gained in developing and utilizing these methods for complicated problems in fluid dynamics includes work in all flow regions, from very low speed (incompressible) to high Mach number flows with shocks and rarefactions. The techniques developed for these studies include the PIC and FLIC methods[27-32] (for several materials in highly contorting, compressible flow), the MAC

method[33-45] (for incompressible flow of fluids with free surfaces), the
ICE method[46-49] (an implicit procedure spanning all flow speeds), and
various hybrid combinations and extensions[50-59] which enlarge consider-
ably the scope of investigations that can be undertaken. In addition
Group T-3 has developed techniques for the inclusion of turbulence
effects.[60-63] All of these resources and experiences will be brought
to bear in the development of the present numerical solution techniques
and computer codes.

B. Neutronics

Heat is generated within a nuclear reactor by two processes, fission
and decay of radioactive nuclides. The distribution of fission heating
follows closely the fission reaction rate, which is given by the product
of the instantaneous neutron distribution and the fission cross section
integrated over all neutron energies. The decay heat, however, de-
pends not on the instantaneous neutron population but on the fission
history of the reactor. During normal operating conditions and during
any accidental excursion in which the reactor is supercritical, the
fission process is the dominant mode of energy production. Decay heat
is of primary importance only when the reactor is shut down neutronically.

Accurate prediction of the rate at which heat is being produced
in a reactor is an important input to the fluid dynamics methods dis-
cussed in the previous section of this report. Because the secondary
criticality problem involves one or more transitions between sub- and
super-critical reactor configurations, both decay and fission heating
may be important. In this section we will discuss methods for solving
the more difficult problem of predicting the fission heating.

The equation governing the distribution of neutrons within a nu-
clear reactor is the time-dependent neutron transport equation. This

equation is often replaced in reactor physics calculations by the less accurate diffusion equation, which is easier to solve. Furthermore, the time dependence of the solution is often treated by means of the point kinetics approximation, in which the spatial shape of the neutron flux is assumed to be independen. ₒf time. Point kinetics methods can be applied to either the transport or diffusion equation.

It is clear from results presenteu in Sec. II.B that transport theory methods must be used to obtain accurate neutron distributions , in the complicated geometrical configurations that are likely to occur when large core motions are permitted. Time-dependent transport theory methods will be required during periods when the reactor is supercritical, that is, when the neutron population is sufficiently large that significant fission heat is generated. When the reactor is neutronically shut down and fission heat is negligible, accurate predictions of the neutron distribution are a waste of time. It is essential, however, that a periodic check be performed to guarantee that the reactor is indeed far subcritical and that no supercritical excursions have been overlooked. Such checks can be made with steady state transport calculations or by occasional time-dependent calculations with large time step sizes. Because a time-dependent transport capability must be provided to treat the supercritical excursions, we will utilize time-dependent transport methods over the entire period of interest, with an automatic adjustment of time step sizes according to the importance of the neutronic behavior of the reactor.

A number of time-dependent transport methods have been developed at Los Alamos. The one-dimensional TIMEX code[64] uses a very fast explicit method for differencing the time variable. The accuracy of this method is improved through the use of two acceleration techniques known as exponential extrapolation and coarse mesh rebalance. All

methods used in TIMEX are capable of being generalized to the two-dimensional (r-z) geometry that is of interest in the secondary criticality problem. The exponential extrapolation method is likely to be particularly well suited to this problem. The two-dimensional (r-z) geometry code TRANZIT[65] uses a less stable centered differencing of the time derivative in the transport equation. This code differs from TIMEX in that iterative methods must be used to solve these centered difference equations at each time step.

In the remainder of this section we present two methods for solving the time-dependent neutron transport equation. Both of these methods utilize the same fixed, Eulerian spatial grid that is used by the fluid dynamics methods discussed above. The use of a fixed mesh by both neutronics and fluid dynamics methods eliminates a costly conversion between Lagrangian and Eulerian meshes and is a major advantage of the methods presented here. The final paragraphs of this section deal with the problems of generating cross section sets as a function of time for use in these transport theory methods.

The time dependent, multigroup neutron transport equations can be written in operator notation as

$$\underline{V}^{-1} \frac{\partial \Psi}{\partial t} = \underline{B}\Psi + q,$$

subject to the initial condition $\Psi(0) = \Psi_0$. The vector Ψ contains the unknown angular fluxes in each energy group as a function of time t, position $\underline{r}$, and direction $\underline{\Omega}$. The diagonal matrix $\underline{V}$ contains the neutron group velocities, the vector q contains inhomogeneous sources and sources due to delayed neutron precusors, and the linear operator $\underline{B}$ takes the standard form

$$\underline{B}\psi = (-\underline{L} + \underline{S})\,\psi$$

$$(\underline{L}\psi)_g = \underline{\Omega} \cdot \nabla\psi_g + \sigma(\underline{r})\psi_g$$

$$(\underline{S}\psi_g) = \sum_{g'} \int d\underline{\Omega}' \; K(\underline{r};\; g',\underline{\Omega}' {\to} g,\underline{\Omega})\psi_{g'}(\underline{r},\underline{\Omega}').$$

The subscript g appearing above denotes the g'th component of subscripted vectors.

In the above equations the operator $\underline{L}$ represents the loss mechanisms of the transport equation. The term $\underline{\Omega} \cdot \nabla\psi_g$ represents loss due to neutron streaming, and the loss due to scattering and absorption is given by $\sigma(\underline{r})\psi_g$. The operator $\underline{S}$ represents all homogeneous source mechanisms, so that the kernel K should be considered as representing both scattering and fission processes.

We are concerned here primarily with methods for treating the time variable. For this reason we will use standard discrete ordinates methods[66] for the angular variables and the diamond difference scheme[66] or one of the new finite element methods[67] for the spatial variables. With a particular choice of methods, we obtain the following semi-discrete system of differential equations:

$$V^{-1} \frac{d\Psi}{dt} = (-L + S)\Psi + q \quad .$$

The vector now contains the unknown angular fluxes at all mesh points as a function of time only. The matrices V, L, and S are approximations of the operators $\underline{V}$, $\underline{L}$, and $\underline{S}$, respectively.

The above equations can be differenced in many ways. The most stable method is that used by the TIMEX code:

$$V^{-1} \frac{\psi^{j+1} - \psi^{j}}{\Delta t} = - L \psi^{j+1} + S\psi^{j} + q,$$

where the source q can be evaluated at time t_j or t_{j+1} or anywhere in between. In the above equation the flux ψ^j is an approximation of the exact flux $\Psi(t_j)$, and $\Delta t = t_{j+1} - t_j$. The above difference scheme yields an unconditionally stable method, in the sense that arbitrarily large time steps Δt can be taken. Furthermore, this method is explicit (no iteration is required to advance the solution by one time step), because the matrix L can be inverted easily.

Explicit methods are very fast but less accurate than the more time consuming implicit methods. The fully implicit method is given by

$$V^{-1} \frac{\psi^{j+1} - \psi^{j}}{\Delta t} = (-L + S) \psi^{j+1} + q \quad .$$

For a given time step size this method is somewhat more accurate than the TIMEX method but also requires more computing time per step. Because the source term $S\psi$ is evaluated at the new time t_{j+1}, iterative methods must be used to solve the above equation for ψ^{j+1}. If the reactor is subcritical, the fully implicit method has the advantage that, for very large time step sizes, the flux ψ^{j+1} is very nearly the steady state solution $(L - S)^{-1}q$.

It is likely that neither of these methods will be satisfactory for following the rapid transients that occur during a supercritical excursion, in which the flux may change by several decades. Special methods are needed to predict accurately such enormous changes in the flux level. The exponential extrapolation method used in TIMEX or a variation of the quasistatic method in which the flux is represented as the product of a slowly-varying shape function times a rapidly-varing amplitude function will be used for these transients. In

either case, a basic method must be available to correct the exponential prediction of the flux or to calculate the shape function. Either the TIMEX method or the fully implicit method can serve in such a capacity.

In the above discussion we have ignored the effects of changes in cross sections due to changes in the neutron spectrum, material heating, and gross motions of core materials. Cross sections will be assumed to be constant over each neutronics time step Δt and will be given by the reactor configuration currently available from the fluid dynamics calculation. Cross section changes due to gross material motion are easy to account for, because the densities of the various core materials are a primary output of the fluid dynamics calculation. Macroscopic cross sections can be obtained by multiplying a set of microscopic reference cross sections by these densities and summing over all the reactor constituents. The effects of changes in the neutron spectrum and material heating could be accounted for by generating new multigroup microscopic cross section sets for each time step, although such an approach would likely be too expensive and not warranted by the needed accuracy.

It is clear that, during periods when the reactor is neutronically shut down, the primary cross-section changes occur because of material motion. During supercritical transients, however, Doppler broadening of resonances and other cross-section perturbations unrelated to material motion become important, if not dominant. We therefore propose to recompute cross section sets at the beginning of each supercritical transient and as often as necessary during the course of the transient. Cross section sets will not be changed during other periods, except to account for gross material motion. The importance of regeneration of microscopic cross sections will be tested, and the use of more

approximate techniques will be examined. In particular, Doppler reactivity coefficients can likely be incorporated by using an effective absorption cross section.

Delayed neutron precursors enter the above equations for the neutron flux through the source term q. The equations for the concentrations of these precursors are simple and involve no spatial derivatives. These equations are easy to solve, and we will not discuss them here. We do note however, that these precursors are carried along with the motions of the molten fuel. Hence the precursor concentrations must be changed by the fluid dynamics algorithms in accordance with core motions.

We believe that the methods discussed above can give accurate answers to two-dimensional time dependent transport problems in reasonable amounts of computer time. We estimate that a FORTRAN language program using the TIMEX method will require about two or three seconds of CDC 7600 computing time per time step for a problem involving six neutron groups, twelve discrete ordinates and 2000 mesh cells. This estimate was made by determining the time required for a single flux iterate in the TWOTRAN code. We estimate further that no more than 500 time steps will likely be required for most problems. Thus we obtain an upper estimate of about one-half hour of computing time for the neutronics part of a typical problem. We emphasize that optimization of methods and programs would result in a substantial reduction in these computing times.

C. Heat Transfer and Related Topics

A number of difficult heat transfer questions arise in conjunction with the large scale material dynamics problem of interest here. All existing disassembly codes assume an adiabatic system. This assumption may be appropriate because, for most prompt bursts in fast reactors, there

is insufficient time for appreciable heat transfer to take place be-
tween materials. This assumption does not hold for the relatively
long times involved in the large scale dynamics problem. The key heat
transfer problems listed below will be elaborated upon individually:

(1) Freezing of steel and fuel in the lower axial shield,

(2) UO_2-PuO_2 vaporization/condensation rates,

(3) Melting and ablation of steel above the core,

(4) UO_2-PuO_2 sodium heat transfer

    a. with sodium film on structural surfaces above the core,

    b. with bulk sodium located somewhere in the upper plenum-
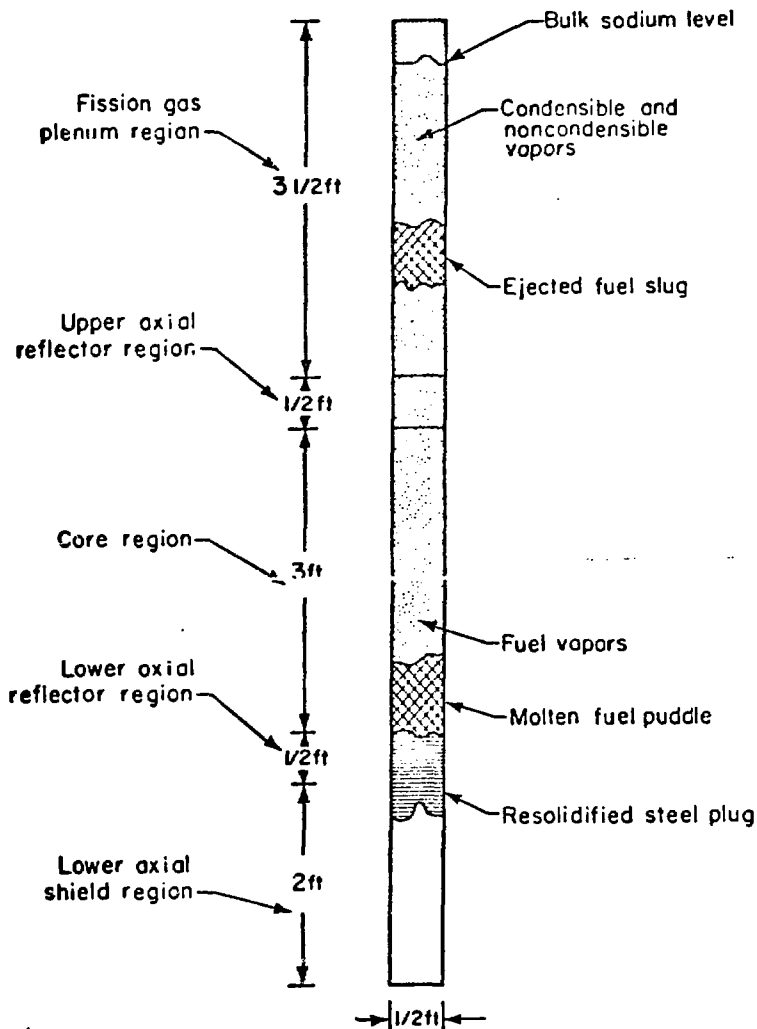   guide tube region

The first problem, freezing of steel in the lower axial shield,
is a pre-disassembly problem which has not been carefully analyzed to
date. The extent to which the lower shield is plugged will be important
in treating the large scale fluid dynamics problem in that area. Some
fuel from the core will attempt to escape through the flow inlet passages
following the first neutronics burst. The amount of fuel which escapes
in this fashion has a direct bearing on the fuel inventory which re-
mains bottled up in the core and is therefore available for secondary
criticality. The flow inlet area is relatively cold ($\approx 500°c$) at this
point (e.g. when molten clad begins to run into the inlet) in the acci-
dent. Freezing of both steel and molten UO_2 is quite likely. Heat will
be continually removed by inlet sodium which is attempting to enter
this lower shield region.

The method used to treat this plugging problem will involve the
geometrical modeling of the inlet region and the application of appro-
priate conductive and convective heat transfer equations. Freezing of

material will effectively reduce the hydraulic diameter and thereby
influence the flow of fuel in the downward direction.

The problem of UO_2-PuO_2 vaporization/condensation rates is impor-
tant in determining the driving pressures which move the core material.
Figure 4 depicts a typical subassembly and shows why rates of conden-
sation and vaporization are important in the large scale material motion
problem. The pressure which drives the ejected fuel slug upward, in
Fig. 4, is UO_2-PuO_2 vapor pressure. The vapor is produced near the sur-
face of the molten fuel puddle at a rate which depends on the pressure
acting on surface. The vapor will condense on the cold subassembly
walls and on structure which remains after the ejected fuel slug passes
by. The condensation rate will depend on the vapor temperature, vapor
density, wall temperature, geometry, and on the presence of nonconden-
sible gases. We expect that, as a result of the tradeoff between vapori-
zation and condensation rates within the subassembly, the ejected slug
will experience a decreasing vapor pressure as it travels up the subassembly
and away from the vapor source. This is an important phenomenon, since
the driving pressures will influence the likelihood for the escape of
the ejected slug from the subassembly. Note that the condensation process
will be important above the slug, as well, since there will be a pocket
of trapped condensible and noncondensible vapors between the slug upper
surface and the bulk sodium level (see Fig. 4). These vapors will create
a back pressure when compressed and act to slow down the slug.

The third problem, melting and ablation of steel above the core,
represents a coupled heat and mass transfer problem which certainly
requires numerical analysis. Figure 5 represents the problem schematically.
Assume that liquid UO_2 which has been ejected from the core comes into
contact with upper plenum structural steel. Due to the very steep

Fission gas plenum region

3 1/2 ft

Upper axial reflector region

1/2 ft

Core region

3 ft

Lower axial reflector region

1/2 ft

Lower axial shield region

2 ft

Bulk sodium level

Condensible and noncondensible vapors

Ejected fuel slug

Fuel vapors

Molten fuel puddle

Resolidified steel plug

1/2 ft

Figure 4

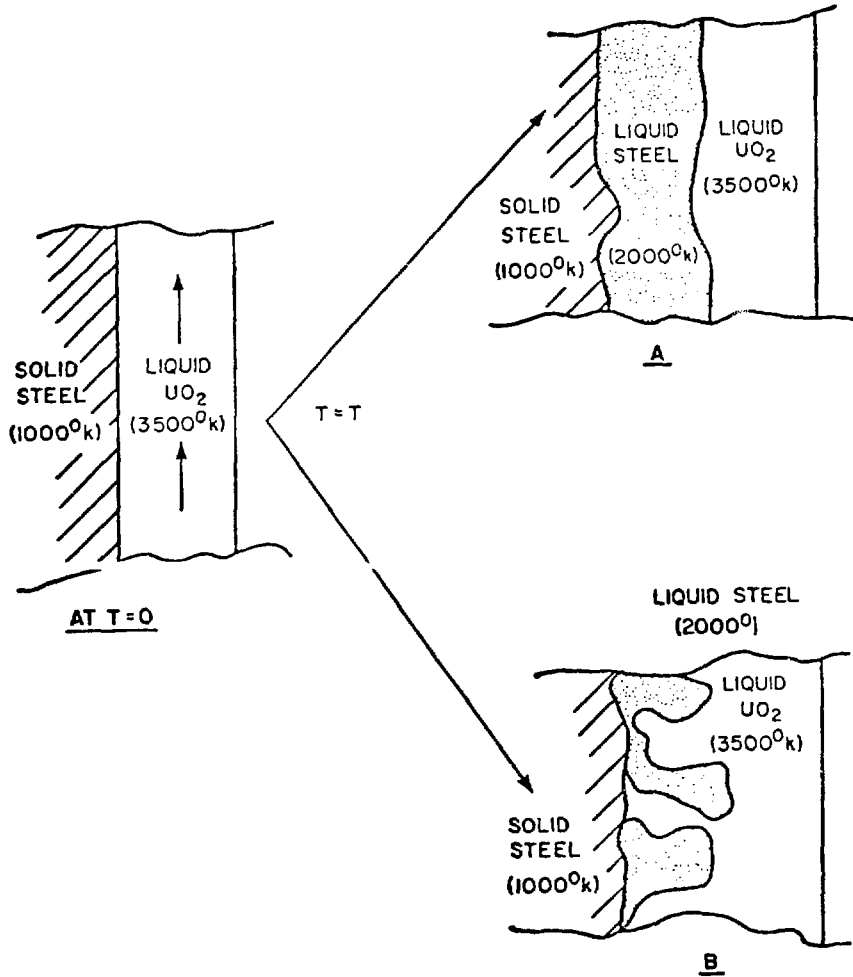Vaporization/Condensation Rates in a subassembly Following Large Scale Disassembly.

Figure 5

Possible Heat Transfer Mechanisms in the
Upper Plenum Region.

temperature gradient between fuel and steel, some surface steel melts immediately. One of two mechanisms A or B in Fig. 5 then comes into play. In situation A, the molten steel forms an insulating layer between fuel and solid steel, and continued steel melting is slow. In situation B, a turbulent boundary layer between fuel and steel is formed, and the steel is mixed with the molten fuel. This means that direct contact between hot fuel and solid steel can continue to occur, and an ablation process will cause rapid steel melting. The mixing of steel and fuel is important from an inertial standpoint, when ejected slug dynamics are calculated. The amount and disposition of steel melted in this fashion will also have a bearing on the neutronics of a secondary criticality. Additional steel involved during core compaction may have a positive or negative reactivity effect, depending on the exact disposition of the steel.

The fourth problem, UO_2-PuO_2 sodium heat transfer, has had more study than the other three problems. The principal result we desire in this work, however, is the effect of fuel-coolant interactions on fuel dynamics. We wish to know whether such an interaction in the upper plenum-guide tube region can drive fuel back down into the core at high velocities. We also wish to know the influence of sodium films which remain on the structural material in the upper plenum. The hot, molten fuel will interact with this sodium in some fashion, and sodium vapors which are produced will have an influence on the fuel slug motion.

Further, it is important to understand the detailed mixing process which occurs when the fuel slug encounters bulk sodium, so that we can predict how much of the fuel slug will be swept out with the accelerating sodium slug as well as the amount and force with which fuel will be driven back into the core. Group T-3 of the LASL is currently developing a method to treat this complicated fluid dynamic, thermodynamic interaction.

D. Equations of State

In any attempt to perform fluid dynamics calculations of more than
a qualitative nature, the equation of state (EOS) of the various materials
involved plays a major role. When the EOS is reasonably well known,
the only problem is in working it into such a form, tabular or analytic,
that the fluid dynamics code can make efficient use of it. If the EOS
has a high degree of uncertainty, as is the case for all the materials--
fuel, sodium, and stainless steel--that must be included in reactor dis-
assembly calculations, then there is the additional task of developing
reliable data from experiment or theory.

Although there exist some data on vapor pressures of the constituent
materials for the temperatures that can be achieved in the laboratory,
they are insufficient to allow calculations of the type we propose.
For relatively serious recriticality events, fuel temperatures of around
10,000°K are not unlikely.[68] A relatively long period of time (seconds)
is conceivably involved in the sequence of events, and consequently sub-
stantial heat transfer may take place between fuel, sodium, and steel.
It is likely that the local sodium temperature will be raised above the
critical point (≈2800°K).[69] There is an intolerable spread in data in
the reactor safety literature in the EOS for both fuel and sodium in
these respective regimes.[70-75] Furthermore, as mentioned in Sec. III.C
of this proposal, stainless steel heating is quite likely, and the rela-
tively high vapor pressure of steel (compared to, say, UO_2) suggests
the strong likelihood of its participation in the disassembly process;
stainless steel EOS data is virtually nonexistent in the reactor safety
literature.

We have already stressed the necessity for EOS data at temperatures
above the readily accessible regime. In Fig. 6 we illustrate schematically
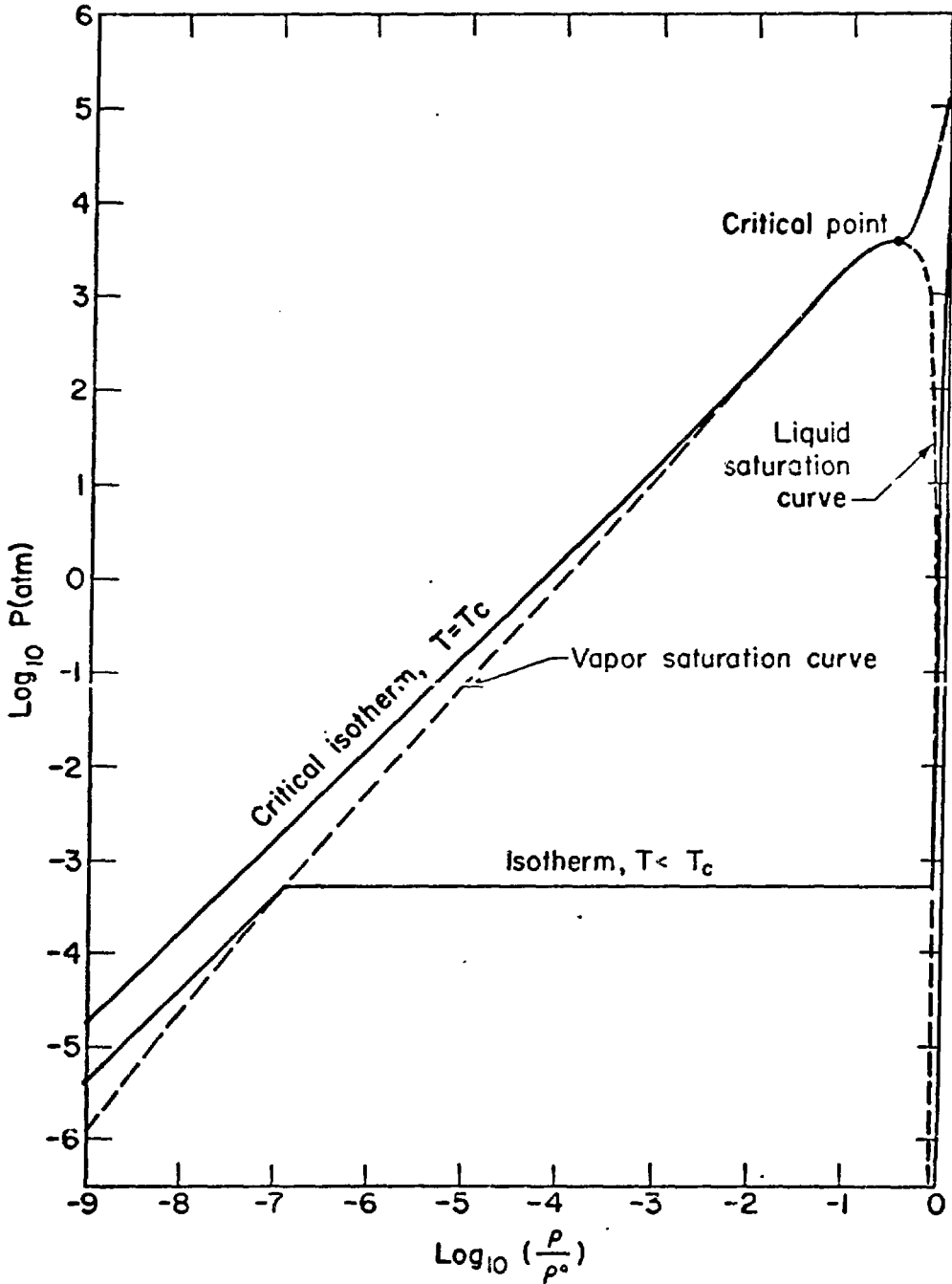
Figure 6

Schematic of Mixed-Phase Region.

the importance of data more refined than vapor pressure alone, namely the vapor saturation curve. The figure depicts the region of mixed liquid and vapor; within the "vapor dome" the pressure at constant temperature is independent of volume. However, after crossing the saturation line to larger volume the pressure drops. If the material pressure is erroneously kept equal to the equilibrium vapor pressure in this regime it is possible that a non-conservative calculation, from the standpoint of recriticality, would result.

Group T-4 of the LASL is developing theoretical techniques[76] for prediction of EOS data in the mixed-phase and imperfect gas regimes from the less-uncertain properties of the solid. When applied to sodium, we obtain vapor pressures in good agreement with experiment and a critical point in reasonable agreement with prediction from available experimental data. We propose to apply the analysis to all materials of interest in the disassembly calculations and to refine the methods to develop as much certainty in the predicted EOS as possible. The results of utilization of the theoretical EOS of a number of materials (not of reactor interest) in "blowoff" calculations, where depiction of the mixed-phase region is important, is now being checked against impulse measurements performed by Group J-15 of the LASL. If later experimental data on reactor materials become available, we will adjust our model to relfect it.

As the fluid dynamics calculations become more refined the question of vaporization rates will be addressed, as will the possible influence of fission-product gas[77,78] on disassembly dynamics.

The LASL has long been an acknowledged expert in the EOS area. Perhaps the most reliable information available, to date, for the EOS of UO_2 has been experimentally and analytically derived at the Laboratory.

Although there have been no plans made as yet, there have been preliminary discussions of the possibility of obtaining UO_2 vapor pressure data using underground weapon test techniques.

Group T-4 has the responsibility for performing theoretical EOS research, constructing and maintaining a computer-based data bank of tabular equations of state in forms suitable for use by hydrodynamics codes. Currently many diverse programs in the LASL use these data.

IV. WORK STATEMENT

The activities described in this proposal consist of several closely correlated efforts. Proceeding simultaneously, their aim will be to develop a progressively more sophisticated computer code for analysis of the neutron kinetics and material dynamics taking place during a hypothetical core meltdown accident in an LMFBR. The initial development of this computer code will include the following efforts:

1. A careful study of the material properties to be expected, including the equations of state, the permeability (inter-penetration) characteristics, heat transfer and phase change descriptions, and the thermodynamics of variable-concentration mixtures.

2. Preparation of a material dynamics computer algorithm. Methods to be used in this initial effort are discussed in Sec. III.A.

3. Testing of the methods discussed in Sec. III.B for two-dimensional time-dependent transport theory.

4. Preparation of a neutron kinetics algorithm.

5. Coupling of the material dynamics and neutron kinetics algorithms into a single code.

The initial computer code, which is to be developed as indicated above, will fulfill two requirements. First, it will be directly applicable to meaningful problems within a short period of time (approximately one year), and second, it will be flexible enough to allow for progressive increase of sophistication and scope of applicability. The first of these goals requires an intensive level of effort, balancing the demands for expediency with those of realism and accuracy. We expect that the initial calculations will be able to present convincing evidence on the subject of LMFBR safety within 18 months of the initiation of this project. The second goal is likewise of importance.

Because of the necessity for investigating a continually broadening scope of LMFBR related configurations and circumstances, it is crucial that the initial computer code admit to progressively greater sophistication.

After the initial computer code has been written and the initial tests and studies performed, we plan to build in a continually enlarging scope of physics and numerical methodology, in keeping with the advancing concepts of design and technology that can be expected in this field of reactor development.

V. PERSONNEL

Kaye D. Lathrop will serve as person-in-charge of the project, and Wm. H. Reed will be principal investigator. Personnel of Groups T-1, T-3, and T-4 of the Theoretical Division of the Los Alamos Scientific Laboratory will participate in the project. These personnel include:

Neutronics

Dr. K. D. Lathrop: T-1 group leader, author of one- and two-dimensional transport codes, and author of publications in the fields of reactor physics and transport theory.

Dr. W. H. Reed: T-1 staff member, numerical analyst, and author of time-dependent and triangular mesh transport codes.

Fluid Dynamics

Dr. F. H. Harlow: T-3 group leader and author of widely-used fluid flow methods.

Other T-3 personnel will include C. W. Hirt, T. D. Butler, and B. D. Nichols.

Equations of State

Dr. J. F. Barnes: T-4 group leader and expert in equations of state.

General Physics

Dr. J. E. Boudreau: T-1 staff member, expert on reactor safety and secondary criticality.

VI. COST ESTIMATE

	FY75	FY76	FY77	FY78
Man Years				
A. Scientific	8	8	8	8
B. Other	0	0	0	0
Costs ($1000)				
A. Direct Salaries	208.4	220.9	234.2	248.2
B. Materials & Services*	67.8	71.9	76.2	80.8
C. Indirect Costs	122.0	129.3	137.1	145.3
Total Costs	398.2	422.1	447.4	474.3
Equipment Costs ($1000)				
A. Obligation	0.0	0.0	0.0	0.0
B. Costs	0.0	0.0	0.0	0.0

*Includes computer costs.

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