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Title: The Simulation of a Criticality Accident Excursion Occurring in a Simple Fast Metal System Using the Coupled Neutronic-Hydrodynamic Method
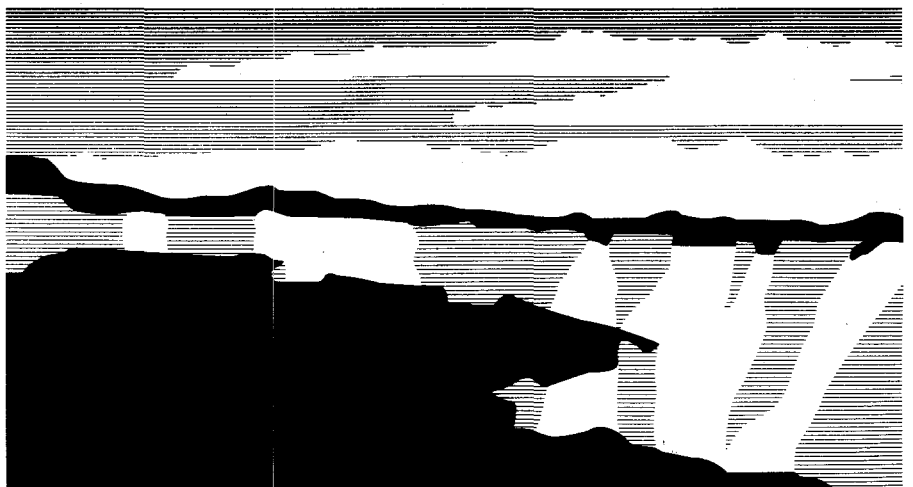
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Outline

The Simulation of a Criticality Accident Excursion Occurring in a
Simple Fast Metal System Using the Coupled Neutronic-Hydrodynamic Method

INTRODUCTION

The purpose of this section is to demonstrate the methodology for analyzing a criticality accident scenario occurring in a simple fast metal system using the coupled neutronic-hydrodynamic method[1]. The coupled neutronic-hydrodynamic method is useful for analyzing excursions which are characterized by very short power periods and high power levels caused by a large and rapid insertion of reactivity. The transients are quenched by reactivity feedback caused from materials motion and high temperatures generated by the excursions themselves. The neutronic-hydrodynamic coupling is illustrated as follows: The reactivity in a nuclear system suddenly increases, causing increased fissions. These fissions generate heat which, in turn, generates pressure sufficient to cause materials motion and increased temperatures, which affects the reactivity of the nuclear system.

A step by step approach will be used to illustrate the creation of a coupled neutronic-hydrodynamic code which can calculate total energy generation and kinetic energy yield during a criticality accident excursion. The last Godiva-I criticality accident will serve as our illustrated example.

HISTORY OF CRITICALITY EXCURSION STUDIES AT LOS ALAMOS USING THE COUPLED NEUTRONIC-HYDRODYNAMIC METHOD

Over the years at Los Alamos, various codes have been developed to study excursions in nuclear assemblies, critical experiments, and criticality accident scenarios using the coupled neutronic-hydrodynamic method. Development of the calculational technique known generally as the "coupled neutronic-hydrodynamic method" proceeded only as rapidly as reliable computers became available. It was not until the early 1950s under the guidance of Ernest W. Salimi and Conrad Longmire of Los Alamos that working codes were created to couple together the differential equations for thermodynamics, material motion, and neutron transport with rapidly changing reactivity. Each code was developed to be an improved version of its predecessor. The codes were (listed in chronological order) the "detailed method," the Reactor Accident code (RAC)[2], the Pajarito Dynamics code (PAD)[3], and, most recently, the MRKJ Reactor Transient code[4].

The first criticality accident analysis application was performed in 1957 subsequent to the accidentally large power excursion in the original Lady Godiva reactor[5] (Godiva-I). Success in reproducing the data from controlled (nondamaging) power excursions and both the thermal energy release and a measure of the damage energy of the last Lady Godiva accident led to more elaborate studies and code development using the coupled neutronic-hydrodynamic method. Other projects and experiments that were planned and analyzed using these codes include the KIWI-TNT[6] experiment, Snaptran[7] series of experiments, and the KEWB[8] series of experiments.

History of Godiva-I or "Lady Godiva"

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History of Godiva-I or "Lady Godiva"

The Godiva-I assembly was created in the early 1950s to be as nearly a sphere of unreflected uranium metal as was possible. The mass of about 55 kg of 93% enriched uranium metal was made in several parts and was assembled by remote control. Figure 1.0 is a photograph of the unassembled Lady Godiva. The supporting structures were light and innocuous to neutrons so as to not perturb the measurement of the critical mass of enriched uranium; it is illustrated in Figure 2.0. The intent of the program was to provide a precise experimental test of neutron transport calculational methods for determination of reactivity and critical mass.

Given the completion of this program, the equipment associated with this critical assembly was modified to allow transient (or pulsed) experiments during which a known reactivity was added rapidly and the response of the assembly and release of energy and neutrons was studied. By about the mid-1950s the addition of reactivity was sufficient to exceed prompt critical by a small amount, with the result that very short period transients (tens of microseconds) were observed.[10] In this early work, the alphas achieved were as large as $8x10^4$/sec.

For these transient experiments with the Godiva assembly, in a typical pulse, the assembly temperature rose by about a hundred degrees, and the metal assembly expanded by a small amount (a few tenths of a mm), sufficient that the negative feedback from increased leakage of neutrons would change its reactivity to below prompt critical. The energy release was a few x 10^{15} fissions, or a few tenths of a megajoule. The energy release would vary linearly up to an alpha value of about $7x10^4$/sec. The expansion of the assembly occurs fast enough to accommodate the energy deposition, as in a quasi static expansion.

However, in the operation of the Godiva assembly with an alpha larger than about $7x10^4$/sec the fission energy deposition in the assembly begins to rise more rapidly than linearly.[10, 11] In this transition region, the assembly is creating energy at a rate faster than the uranium can expand to accommodate the deposition of the energy (in the form of heat); the expansion is no longer in a quasi static equilibrium. This increase in the yield curve is due to inertial effects, and these inertial effects cause stresses to develop in the assembly material. The metal first is in compression as the temperature rises but later is in tension as the system expands; the material is held together by tensile strength of the metal. That is, the metal of the assembly is being stressed by the energy deposition, but remains within the elastic limit of the material. A "ringing" of the outer surface has been observed subsequent to the completion of each transient experiments.[11]

The significance of the "compression-tension" effect became much more evident in 1957[12]. An error in preparations for an experiment led to a shorter period (larger alpha) and larger energy release than had been planned. The period was about 5 microseconds (alpha = $2x10^5$/sec) and the energy release was about $1.2x10^{17}$ fissions. Damage to the assembly and supporting was evident, the central "burst" rod had softened and ruptured. The central volume was close to the melting temperature and had softened and expanded. Figure 3.0 is a photograph of the Godiva-I assembly after the accident.
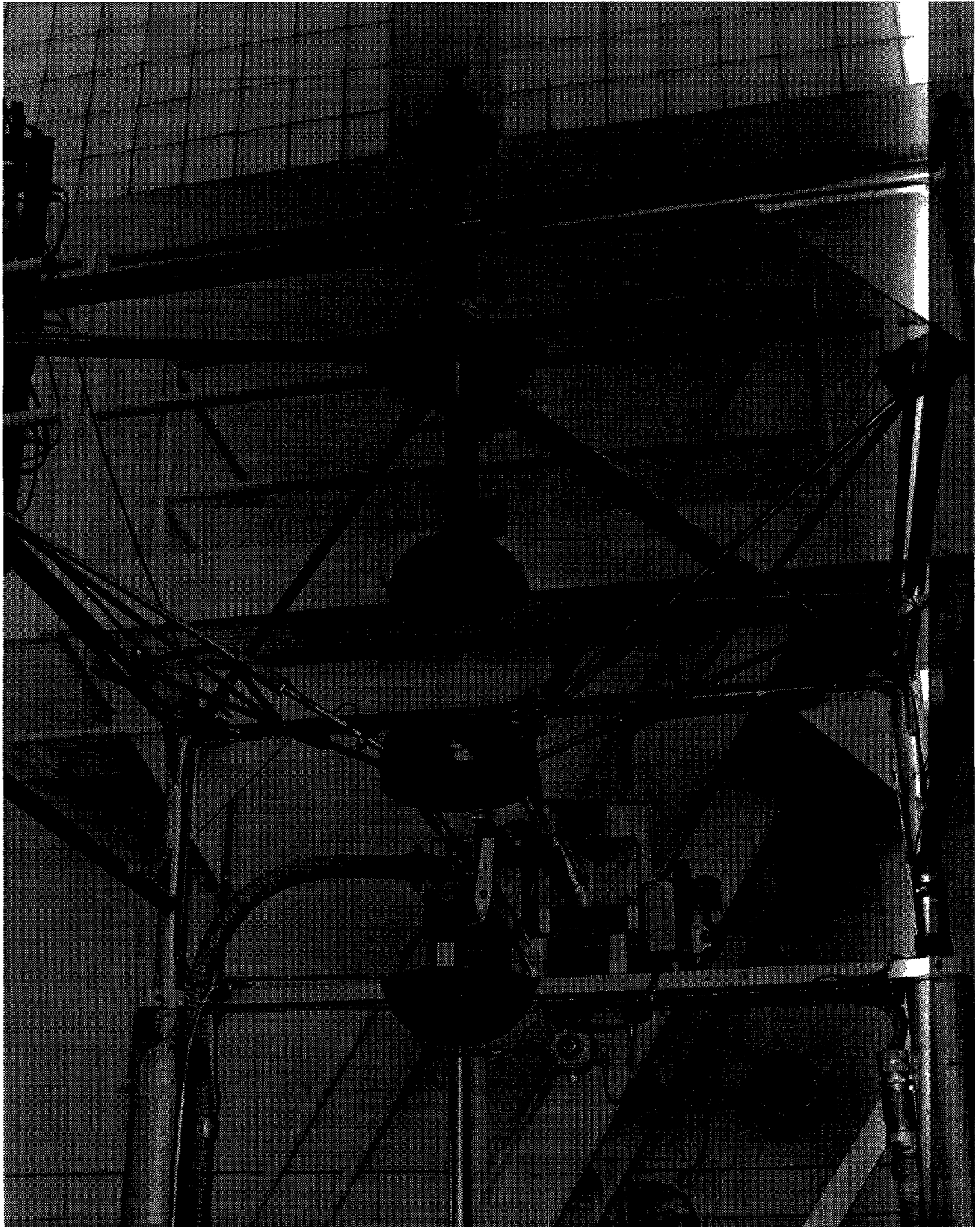
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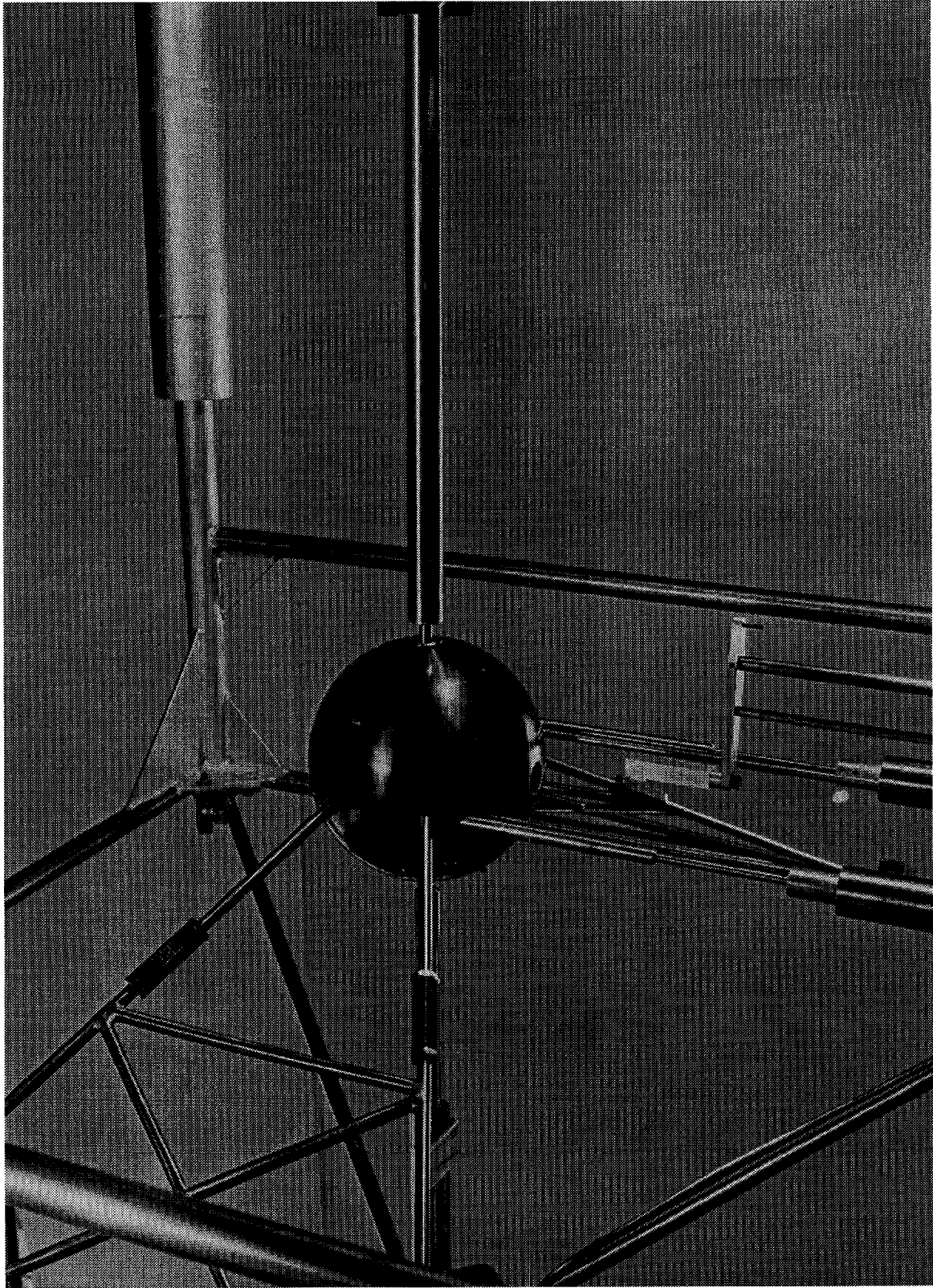*Figure 1.0. Photograph of the unassembled Lady Godiva.*

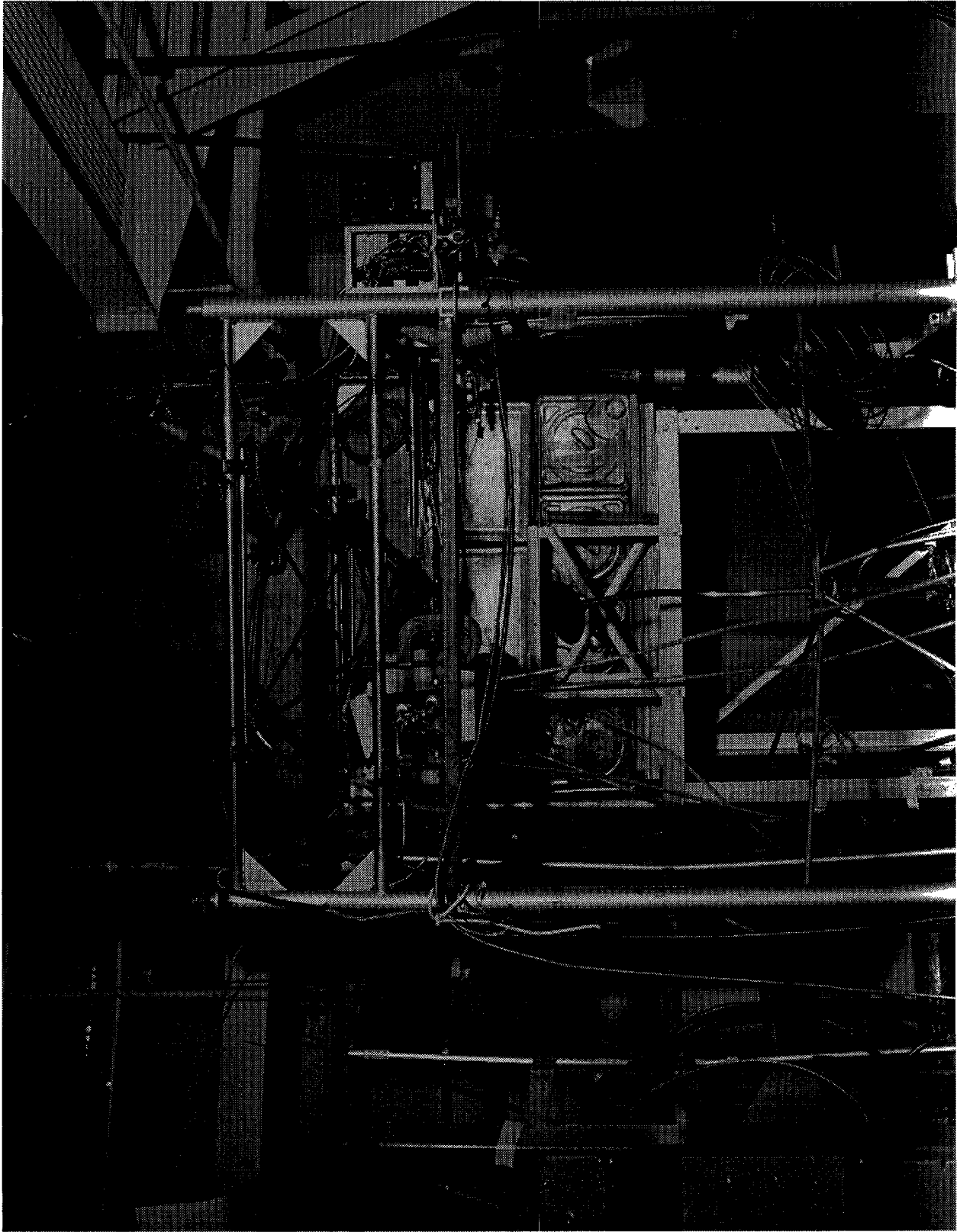*Figure 2.0. Close-up photograph of the assembled Lady Godiva.*

Figure 3.0. Photograph of the Lady Godiva assembly after the accident in 1957.

Basic Tools

Simulation of a reactor excursion using the coupled neutronic-hydrodynamic method requires the construction of an idealized reactor model and the solution of the coupled equations governing the motion of the materials and the neutron transport phenomena. The word hydrodynamic is used in the context that the motion of materials is governed by the equation of motion of a compressible fluid.

To create a code that can perform a dynamic analysis using the coupled neutronic-hydrodynamic method, the following basic tools or information is needed:

1. A neutron transport code is needed that can estimate k_{eff} or "alpha" of the nuclear system. "Alpha" can be considered the inverse reactor power period or a measure of how fast energy can be deposited in the system. If the neutron transport code can only perform k_{eff} calculations, an estimate of the neutron lifetime l in the nuclear system is needed. Then, substitution of the approximation $\alpha = \frac{k_{eff} - 1.0}{\ell}$ can be used.

2. Empirical formulas or tables for equation of state data and other thermal properties of the materials that make up the nuclear assembly are needed.

3. Empirical formulas or tables for hydrodynamic properties of the materials that make up the nuclear assembly are needed.

To illustrate the use of the coupled neutronic-hydrodynamic method to study a criticality accident scenario in a fast metal system, we will look at the last Godiva-I accident.

INITIAL MODEL ASSUMPTIONS

To begin our analysis of the final Godiva-I accident, we need to state the initial assumptions that we will use to construct our idealized model of the Godiva-I assembly. The basic assumptions are:

1. The Godiva-I assembly will be modeled as a solid sphere of 93% enriched U-235 metal. Spherical coordinates in one-dimension (radial) will be used to set up the geometry.

2. The accident excursion will be modeled as if the transient was initiated by a step insertion of reactivity.

3. The initial size of the Godiva-I assembly will be chosen such that its initial alpha value will be equivalent to the estimated maximum alpha value that was achieved during the accident.

4. As the transient begins, all the variable values (power, temperature, pressure, density, etc.) are known.

5. Uranium metal will be modeled such that it has tensile strength.

NEUTRONICS

The neutron transport calculations will be done in spherical coordinates using the one-dimensional discrete ordinates code ONEDANT.[13] The "alpha" or time absorption option of the ONEDANT code will be used in conjunction with a 167 isotope library of Hansen-Roach Sixteen energy group cross sections[14] to perform all the neutron transport calculations.

An initial radial dimension search calculation is done using ONEDANT to find the equivalent size uranium ball that would have an initial alpha value about equal to that estimated for the final accident excursions $(2 \times 10^5/\text{sec})$.

GEOMETRY

A Lagrangian approach will be used to attack the hydrodynamic and thermodynamic portions of the problem. This means that we will divide up the system into small control volume pieces which we will call fluid elements and record the changes that occur to each fluid element as it moves through the system.

Since we are using spherical geometry in one-dimension to create our ideal model of Godiva-I, the system is divided up along the radial axis beginning at the geometric center. Each mesh interval represents a spherical or spherical shell fluid element. Our idealized Godiva-I model will be divided up as shown in Figure 4.0.
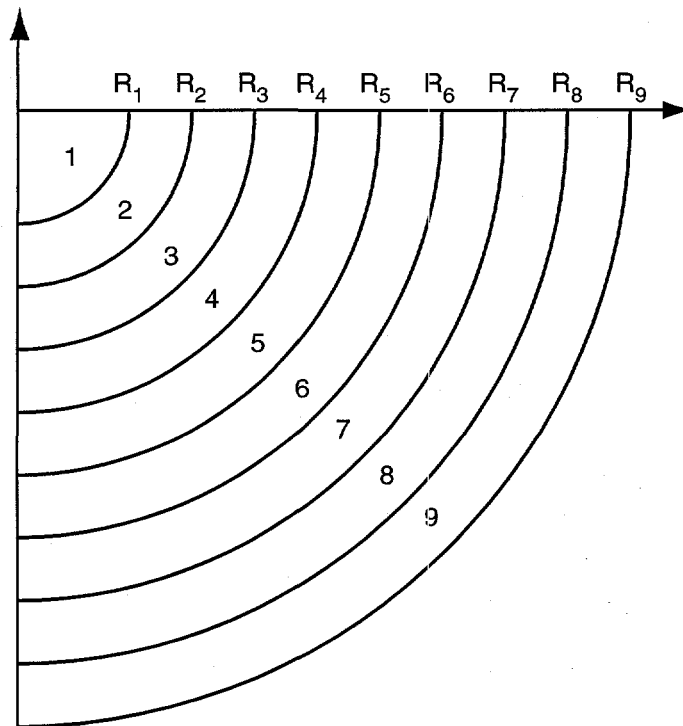

Figure 4.0. Mesh spacing of fluid elements in our idealized Godiva-I model.

The outer radial position of the fluid element surface is the Lagrangian coordinate associated with each fluid element. For example, R_1 is the Lagrangian coordinate associated with fluid element 1. Table 1 lists the initial radial positions of the Lagrangian coordinates for the fluid elements in our idealized Godiva-I model.

Table 1. Initial radial positions of the Lagrangian coordinates associated with each fluid element for the idealized Godiva-I model.

$R_1 = 1.0$ cm	$R_5 = 5.0$ cm
$R_2 = 2.0$ cm	$R_6 = 6.0$ cm
$R_3 = 3.0$ cm	$R_7 = 7.0$ cm
$R_4 = 4.0$ cm	$R_8 = 8.0$ cm
	$R_9 = 8.8230$ cm

GOVERNING EQUATIONS

When the excursion begins, the system is assumed to be fully specified. The subsequent behavior of the system is determined by solving the coupled equations that govern the motion of the materials and the production and transport of energy and neutrons. This allows us to treat the excursion evolution as an initial value problem and record the changes to all the variables as the excursion proceeds. The equations form a set of coupled first order differential equations which can be solved using a fourth order Runge-Kutta integration scheme.[15]

An equation solves for the total power of the system as a function of time:

$$\frac{dP_{ower}}{dt} = \alpha P_{ower}$$

where

P_{ower} = total power of the system,

$\alpha = \alpha_{geom} + \alpha_{feedback}$,

α_{geom} = time absorption "alpha" from the neutron transport calculation which is dependent upon the geometry and isotopic content of material mixtures in the system, and

$\alpha_{feedback}$ = feedback "alpha" which can be used to incorporate difficult to model reactivity effects.

An equation solves for the total amount of energy generated by the system as a function of time:

$$\frac{dE}{dt} = P_{ower}$$

where E = the total amount of energy generation.

8

Each fluid element has its own energy balance equation, equation of state, and set of equations governing its motion. The state variables are assumed to be uniform throughout each fluid element.

The energy balance equation, which was derived from the first law of thermodynamics, is used to find the temperature in each fluid element. The energy balance equation that we will use for uranium metal has the following form:

$$\frac{dT_j}{dt} = \frac{1}{m_j C_{Vj}}\left[P_{ower_j} - \beta_{Tj}B_j T_j \frac{dV_j}{dt}\right]$$

where

T_j = temperature of fluid element j,

m_j = mass of material in fluid element j,

C_{Vj} = specific heat at constant volume of the material in fluid element j,

P_{ower_j} = rate at which fission energy is deposited in fluid element j,

β_{Tj} = bulk modulus of the material in fluid element j, and

V_j = volume of fluid element j.

The individual fluid element power distribution is determined by normalizing the fission rate in each fluid element to the total fission rate of the system and distribute the power accordingly. The total and individual fluid element fission rates are obtained from the neutron transport calculation.

Other terms that account for energy transport between fluid elements (i.e., conduction, radiation heating, etc.) were omitted from the energy balance equation. This approximation works well when modeling an excursion that evolves in a very short time scale because the relative rate of energy deposition due to fission in a fluid element is much larger than the relative rate of energy transport between adjacent fluid elements.

A general purpose linear form for the equation of state (in differential difference form) is used for uranium metal.

$$\Delta P_j = \beta_{Tj}B_j\left(T_j - T_{jref}\right) + B_j \frac{\Delta\rho_j}{\rho_j}$$

where

ΔP_j = condensed pressure change from previous time step calculation in fluid element j,

T_j = temperature in fluid element j,

T_{jref} = reference temperature from which hydrodynamic data values are taken,

$\Delta\rho_j$ = density change from previous timestep calculation in fluid element j, and

ρ_j = density of material in fluid element, j.

This form of the equation of state is a good approximation to use with materials where the bulk modulus is a function of the velocity of sound through the material given by the relation

9

$$B = \rho V_s^2$$

where V_S = velocity of sound through the material.

Equations of motion are used to determine the radial position changes of the Lagrangian coordinates associated with each fluid element. The motion is generated by pressure differences between adjacent fluid elements. Figure 5.0 is a representation of an interface between two adjacent fluid elements.
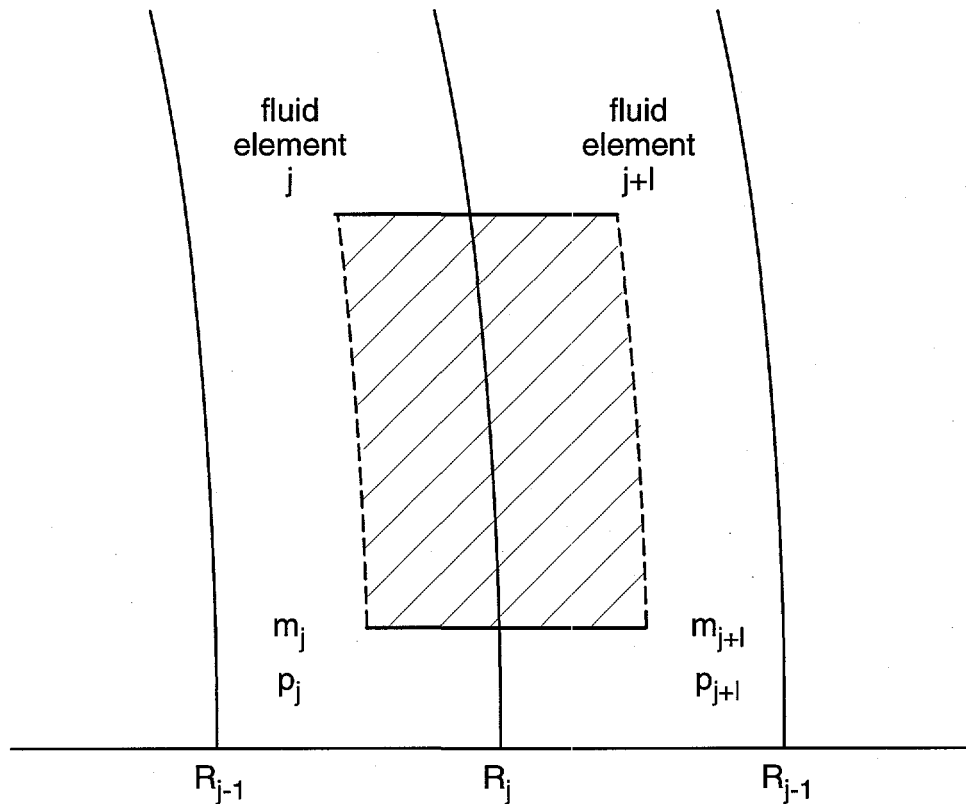

Figure 5. The interface between the adjacent fluid elements.

The physical quantities that are of interest for setting up the equations of motion are:

j_{th} boundary mass = $1/2$ ($m_j + m_{j+1}$),

P_j = total pressure in fluid element j,

P_{j+1} = total pressure in fluid element j+1, and

R_j = Lagrangian coordinate for fluid element j.

The equations of motion are given by:

$$\frac{dv_j}{dt} = \frac{\Delta P_j S_j}{\frac{1}{2}\left(m_j + m_{j+1}\right)}$$

10

and

$$\frac{dr_j}{dt} = v_j$$

where

$\Delta P_j = P_j - P_{j+1}$ = total pressure difference between fluid element j and j+1,

S_j = surface area between fluid elements j and j+1, and

v_j = velocity of the Lagrangian coordinate (or outer surface geometry) of fluid element j.

We will also include in our idealized model of Godiva-I that uranium metal has tensile strength with a yield point. If the total pressure in a fluid element exceeds the yield point, then that fluid element is assumed to be "broken" and no longer has any tensile strength.

A code created using the coupled neutronic-hydrodynamic method is able to examine the partition of fission energy between heat and kinetic energy. The instantaneous kinetic energy of the system is calculated as follows:

$$K.E. = \sum_{j=1}^{n} \frac{1}{2}\left[\frac{1}{2}\left(m_j + m_{j+1}\right)v_j^2\right]$$

where

n = number of fluid elements,

j^{th} boundary mass = 1/2 (m_j + m_{j+1}), and

v_j = velocity of jth fluid element's Lagrangian coordinate (velocity of the jth fluid element's outer surface).

Computational Considerations

Once the idealized model for the system has been constructed, some decisions have to be made concerning the flow of calculations and optimization of calculational run times versus accuracy of results. For our coupled neutronic-hydrodynamic code, the following items need to be determined:

1. How many hydrodynamic calculational cycles are performed per neutron transport calculation?

2. What size time step is chosen to begin the calculation?

3. What criteria is used to determine when to end the calculation?

If the code is written to allow for adjustment of time step sizes in the integration routine, the following items also need to be determined:

1. What is the minimum or maximum time step size one should allow during the calculation?

2. What criteria should be used to determine if the time step size should be adjusted during the calculation?

Figure 6.0 shows the basic flow diagram of calculations that was used to construct our coupled neutronic-hydrodynamic code.
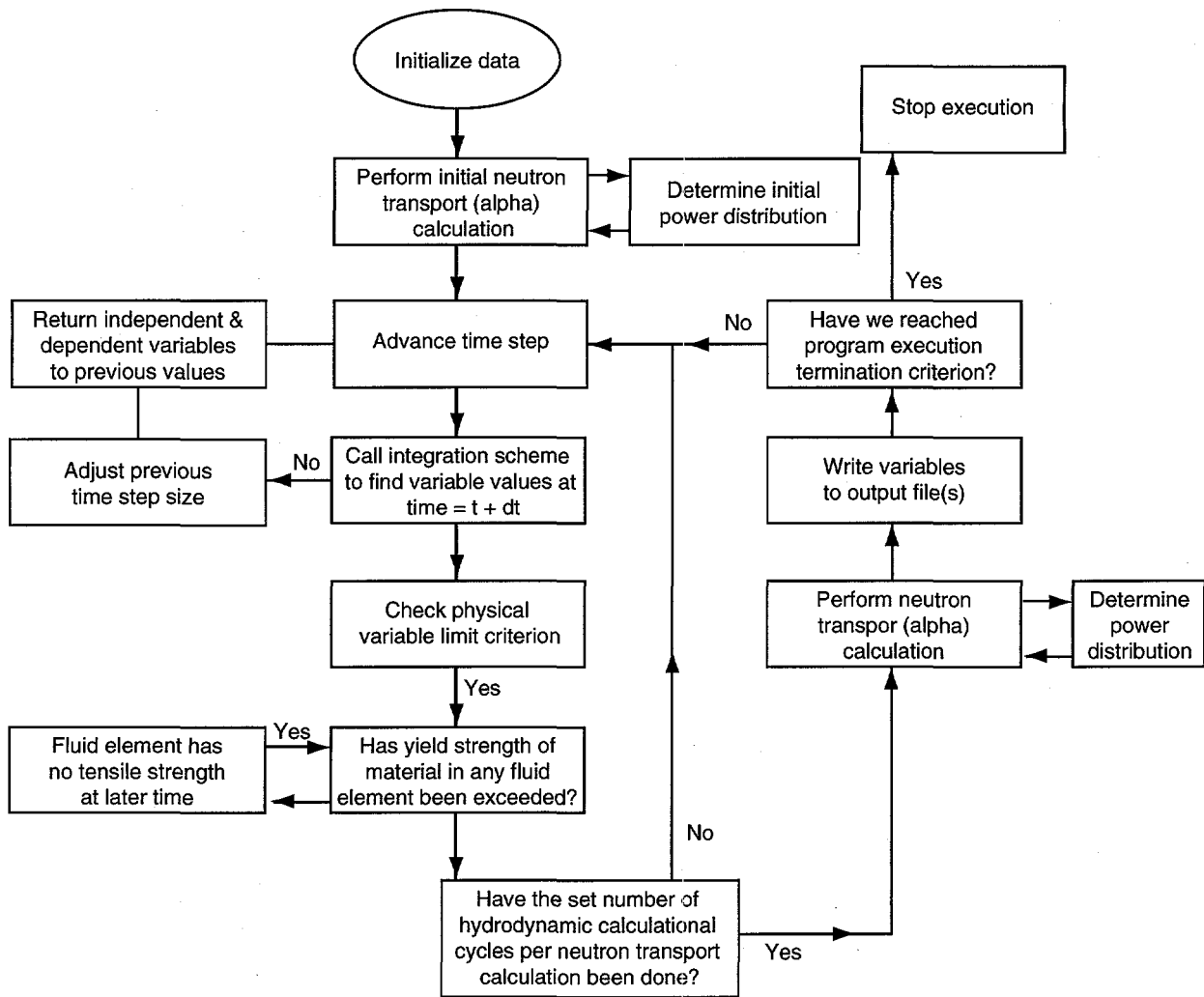
Figure 6.0. Basic flow chart of calculations for a computer code that was developed using the coupled neutronic-hydrodynamic method.

Results

The most important results obtained from an excursion simulation is the total energy generation and an estimate of the maximum attainable instantaneous kinetic energy. Inspection of the state variables allow one to evaluate the validity of the approximations used to create the idealized model of the nuclear system. For example, if the temperature in a fluid element exceeded the melting temperature of the material, then one may want to incorporate some sort of phase change model for that material.

Figures 7.0–9.0 are graphs of state variables and other data obtained from the simulation of the last Godiva-I accident excursion. The MRKJ one-dimensional reactor transient code, which is being developed at Los Alamos for studying transient nuclear systems, critical experiments and criticality accident scenarios using the coupled neutronic-hydrodynamic method, was used to obtain the results.
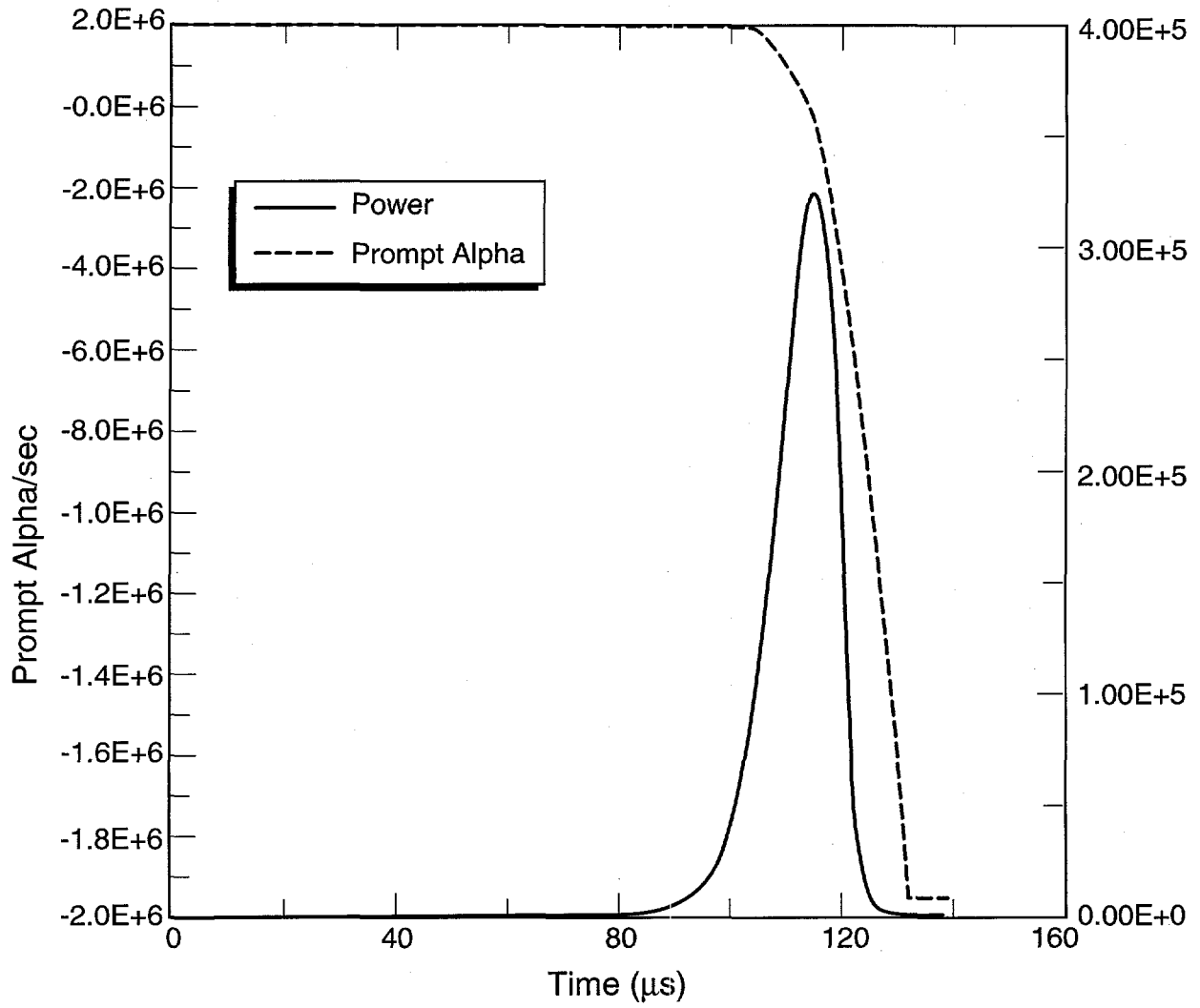
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Figure 7.0. Power and Alpha versus time from the simulation of the last Godiva-I accident using the MRKJ code
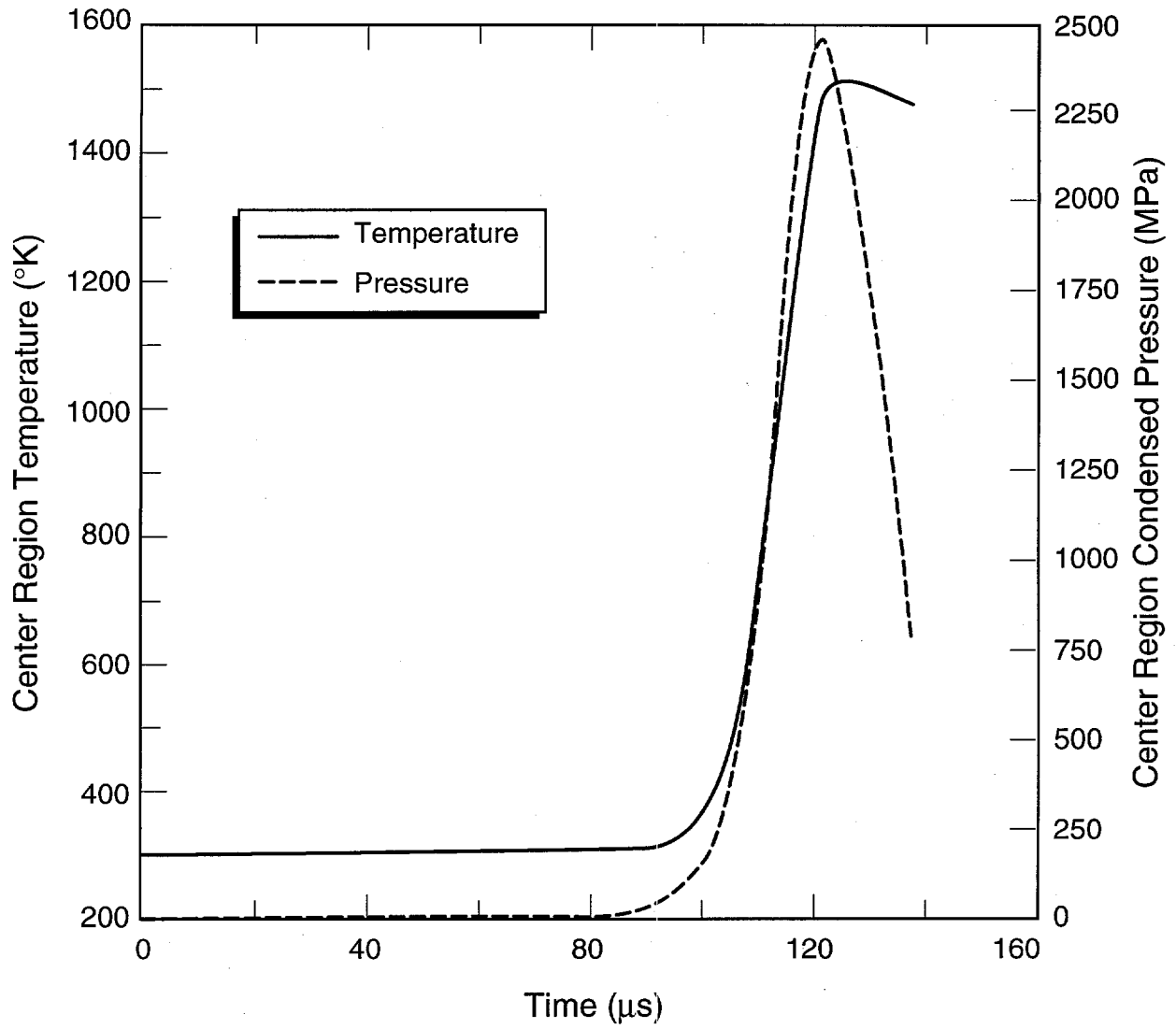
Figure 8.0. Temperature and Pressure versus time for Region I of the idealized Godiva-I model from the accident simulation using the MRKJ code.
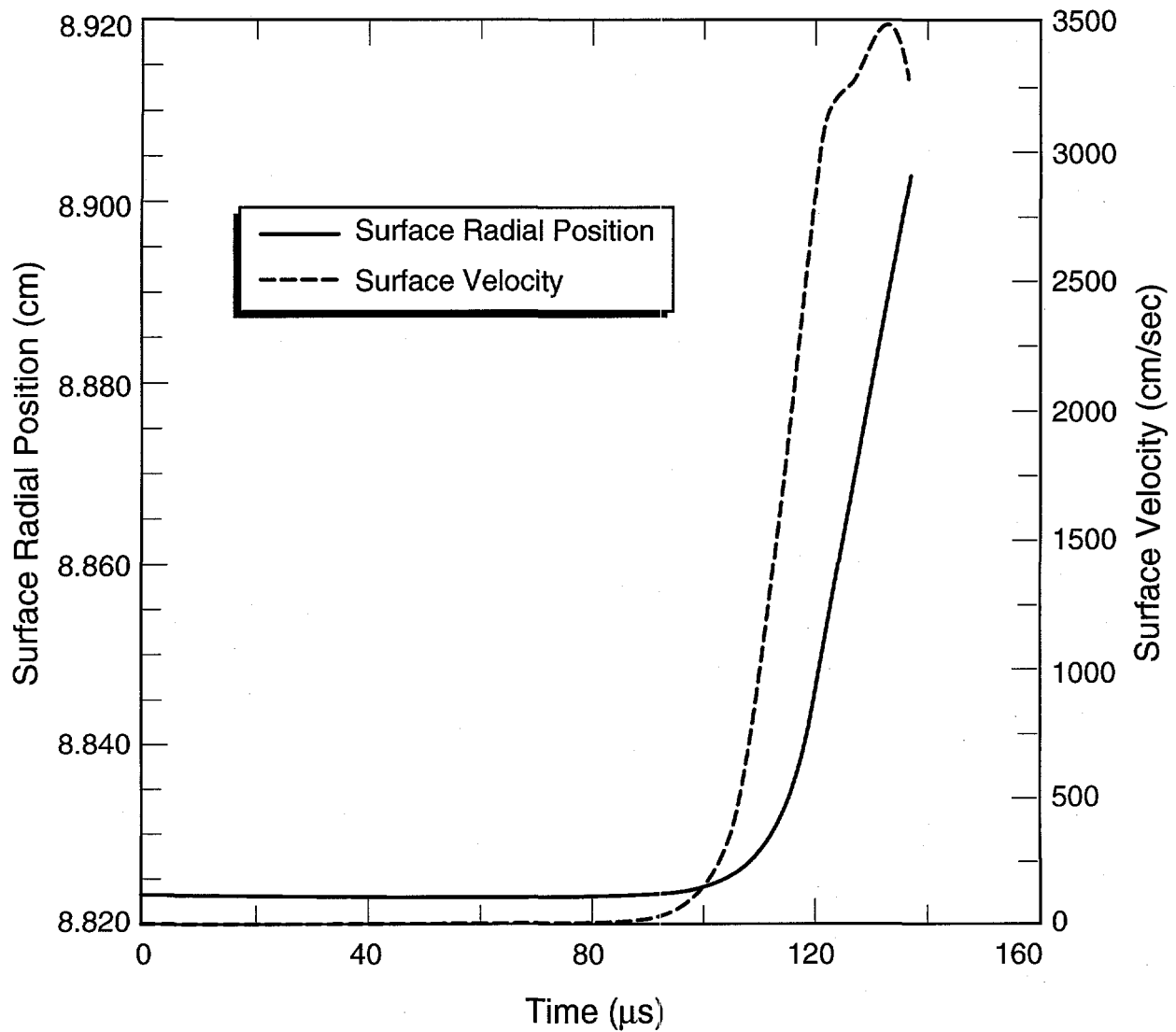
Figure 9.0. Radial position and velocity versus time of the outer surface of Godiva-I from the accident simulation using the MRKJ code.

The total energy generation estimate from our simulation of the last Godiva-I accident was 1.4×10^{17} fissions. The estimated maximum kinetic energy yield was $4. \times 10^{-2}$ MJ. Table 2.0 shows a comparison of the MRKJ code estimates and the real accident estimates.

Table 2.0. Comparison of the MRKJ code and the real accident estimates.

	Accident Estimate	**MRK Estimate**
Total Energy Yield	1.2×10^{17} fissions	1.4×10^{17} fissions
Kinetic Energy Yield	.05 MJ	.048 MJ

15

SUMMARY

Analysis of a criticality accident scenario occuring in a simple fast metal system using the coupled neutronic-hydrodynamic method was demonstrated by looking at the last Godiva-I criticality accident. The basic tools and information for creating a coupled ceutronic-hydrodynamic code were presented. Simplifying assumptions and approximations for creating an idealized model for the Godiva-I system was discussed. Estimates of the total energy generation and the maximum attainable kinetic energy yield are the most important results that are obtained from a coupled neutronic-hydrodynamic code.

With some extra effort, the methodology presented in this paper can be extended to analyze criticality accident excursions in other kinds of nuclear systems (i.e., solution system or other nuclear fuel/moderator/reflector combinations).

DISCLAIMER

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