LA-3683-MS

MASTER

LOS ALAMOS SCIENTIFIC LABORATORY
of the
University of California
LOS ALAMOS • NEW MEXICO

Development of Calculational Methods
for Fast Reactor Safety Analysis at LASL

UNITED STATES
ATOMIC ENERGY COMMISSION
CONTRACT W-7405-ENG. 36

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

All LA...MS reports are informal documents, usually prepared for a special purpose and primarily prepared for use within the Laboratory rather than for general distribution. This report has not been edited, reviewed, or verified for accuracy. All LA...MS reports express the views of the authors as of the time they were written and do not necessarily reflect the opinions of the Los Alamos Scientific Laboratory or the final opinion of the authors on the subject.

Printed in the United States of America. Available from
Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151

Price: Printed Copy \$3.00; Microfiche \$0.65

LA-3683-MS
UC-80, REACTOR
TECHNOLOGY
TID-4500

CISTI PRICES

H.C. \$ 2.00; MN 65

LOS ALAMOS SCIENTIFIC LABORATORY
of the
University of California
LOS ALAMOS • NEW MEXICO

Report written: April 24, 1967

Report distributed: May 17, 1967

**Development of Calculational Methods
for Fast Reactor Safety Analysis at LASL**

by

Carl A. Anderson, Jr.

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

PREFACE

The material in this report was presented orally at the Liquid Metal Fast Breeder Reactor Program Office Seminar on Computational Methods for Fast Reactor Safety Analysis at Argonne National Laboratory on October 4, 1966. Inasmuch as the proceedings of that meeting have not been, and will not be, published, the material is being issued in this form for reference purposes.

ACKNOWLEDGMENT

The author expresses his appreciation to those persons cited herein for their kind permission to make use of published and unpublished material in this cursory review of calculational methods developed at the Los Alamos Scientific Laboratory.

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

I. THE MAXIMUM CREDIBLE ACCIDENT (MCA)

In fast reactor safety analysis, considerations of the maximum credible accident often overwhelm all other safety considerations, and the maximum credible accident calculations often degenerate (unfortunately) into excursion calculations. Most of the Seminar attendees are familiar with the AX-1 code¹ developed by ANL and LASL for excursion calculations, so that will not be discussed. Consider, instead, the simpler RAC code² of C. G. Chezem and W. R. Stratton, which is currently being improved by D. M. Peterson.³ RAC, although developed for the graphite KIWI reactors and successfully applied to the KIWI-TNT experiments, is equally applicable to fast reactors. The original version of RAC only performed calculations for a one-dimensional slab. The code has been improved to consider a 1-D slab, sphere, or infinite cylinder or a two-dimensional finite cylinder. The graphite equation of state used for the KIWI calculations is in a subroutine and is readily altered for consideration of other materials. Thus, Peterson is now using RAC to calculate GODIVA-II excursions; the only difficulty in the application is the necessity to make a wild guess at the equation of state (a difficulty common to most excursion calculations).

An apparent shortcoming of RAC in comparison with AX-1 is the fact that the former merely uses an initially specified flux weighting in the reactivity calculations, while AX-1 performs successive S_4 transport theory calculations. Yet, it may not be a great advantage to use a sophisticated neutronics model as part of a calculational procedure in which something as important as the equation of state is so poorly known. A RAC-DAC combination may be a satisfactory solution.

DAC⁴ is the Data Analysis Code developed by B. M. Carmichael. In this code, both real and adjoint calculations are first performed in two dimensions, using either the DDK S_n code or the CRAM diffusion code. The real and adjoint fluxes are then input to DAC, together with group cross-section data, data from the Data Preparation Code (DPC)⁵

describing the reactor system, and data concerning the perturbation. DAC can provide the effective delayed neutron fraction, neutron lifetime and the reactivity worth of unit density of each element and material contained in the reactor at every mesh point in the system. DAC also provides distributed temperature coefficient data; i.e., it computes reactivities due to perturbations in material densities or microscopic cross sections caused by temperature changes at each mesh point. Thus, arbitrary material displacements arising from thermal expansion or such cross-section perturbations as the Doppler effect may be treated rigorously within the framework of two-dimensional first order perturbation theory.

Use of DAC in conjunction with RAC will allow for better reactivity calculations than the original RAC code could perform, and should require much less computer time than the succession of S_4 calculations required for AX-1. Considering the small volumetric increase needed to terminate a reactivity excursion, a perturbation calculation should be satisfactory.

A difficulty in excursion calculations mentioned here and in all similar meetings is the poor knowledge of the equation of state of the reactor core at high temperatures and pressures. While this difficulty does not fall under the heading of "calculational methods," it is undoubtedly of interest to attendees of this Seminar. The equation of state is usually obtained by prediction of the critical point followed by application of the so-called "law" of corresponding states (which is not a law at all, but a rule-of-thumb). This importance of the equation of state in excursion calculations has been pointed out by many authors (such as Nicholson⁶ and Wolfe, Friedman and Riley⁷), but experimental corroboration of the assumed equations of state has been limited to the very low temperature, low pressure region of p-v-E space. Thus, for example, Méyer and Wolfe⁸ predict the equation of state of UO_2 to 40,000°K and 40,000 atm, and Menzies⁹ does so to 20,000°K and 20,000 atm, but no data above 2800°K are available for corroboration. It is possible that dynamic high-pressure equation of state measurement techniques may be adapted to provide the necessary experimental p-v-E data to evaluate the predictions. This technique¹⁰ employs detonation of an explosive

which, either directly or by means of a driver plate, generates a shock wave through the material of interest. Measurement of the shock wave velocity and particle velocity, and analysis using the laws of conservation of mass, energy and momentum, enable one to determine the equation of state of the material at the shock wave. Normally, this technique is used at pressures up to several million atmospheres and increases in temperature up to only a few hundred degrees Kelvin. Use of a material of relatively low shock impedance results in a lower pressure rise and a higher temperature rise, and it is this modification of the technique which holds forth the promise of obtaining equation of state data in the p-v-E domain of interest for fast reactor accident analysis.

II. FAST REACTOR SAFETY PROBLEMS LESS CATASTROPHIC, AND FAR MORE CREDIBLE, THAN THE MCA

Neutron kinetics, hydrodynamics, and heat transfer are of interest insofar as they bear on the initiation of the maximum credible accident (e.g., core meltdown) and also for more likely, less serious problems such as fuel element cladding failure or thermal shock to heat exchangers. Fast reactor safety analyses at LASL have tended to bear more on these more likely problems than on the MCA.

A. Neutron Kinetics

Because of the very small prompt neutron generation time in a fast reactor, calculation of the kinetic behavior of a fast reactor by the common forward-step finite difference approximation of the point kinetics equations requires very small time steps, and, consequently, very long computer running times. This is of particular disadvantage when the neutron kinetics calculation is applied to moderate transients such as those initiated by power demand or loss of flow. J. C. Vigil¹¹ has applied the method of continuous analytic continuation to the nonlinear reactor kinetics equation. Basically, the method consists of expanding those variables which are analytic

functions of time in Taylor series over successive intervals in the time domain. The method yields a definitive criterion for the magnitude of each time step, each of which can be much larger than the prompt neutron generation time. The use of this criterion guarantees that the error in the results increases at most linearly with the number of time steps so that specification of a maximum allowable error defines the maximum truncation error in each Taylor expansion. Figure 1 shows the results of application of this technique to the Godiva reactor, a fast, bare U-235 sphere. The disagreement between experiment and calculation for large values of initial inverse period is due to the mechanical inertia of the assembly, which was not considered in this calculation. Figure 2 illustrates the application of a continuous analytic continuation calculation to the SPERT-I reactor, a heterogeneous, water-moderated thermal reactor. The agreement between calculated and experimental results is good.

The DAC code, mentioned above in connection with the MCA excursion problem, is, of course, also applicable to other safety calculations.

K. D. Lathrop and B. G. Carlson have studied the problem of extending the S_n calculations to the time domain,¹² and foresee no insuperable problems in such extension. A small amount of such extension has been done but has not been reported. A decision on whether to proceed with development of a time-dependent S_n code will be made in the near future.

B. Heat Transfer

R. Axford has derived¹³ an analytic solution for the transient temperature response of cylindrical fuel rods and associated coolant (which can be extended to other--e.g., plate--geometry), considering time-and-space dependence of power density, coolant temperature and coolant speed. This analytic solution, employing finite Hankel transforms, has several advantages over the more common finite-difference approximation calculations such as that employed in the FORE code.¹⁴ First, the approximations inherent in any finite difference approximation are avoided, and second, the computational time is much less for the same mesh size. Axford's method also requires much less computer storage space.

Fig. 1. Comparison of Calculated and Experimental Peak Fission Rate as a Function of Initial Inverse Period for GODIVA Reactor. (From Ref. 11)

PEAK POWER (MW)

Fig. 2. Comparison of Calculated and Experimental Peak Power as a Function of Initial Inverse Period for SPERT-I Reactor. (From Ref. 11)

The natural convection process is important for the safety of a LMFBFR, particularly in the event of a pump or loop failure which could result in fuel meltdown. Nonetheless, there is no straightforward method for predicting the behavior of a particular system involving natural convection. B. Goplen and J. Cleary¹⁵ are developing a computer program for prediction of LMFBFR system temperatures and natural convection flow rates. The program is aimed particularly at the transient condition following a total loss of forced convection, but will also be applicable to steady-state natural convection. The primary purpose of the attendant experimental study will be to determine the hydraulic-thermal relationships for a natural convection system, particularly with regard to film coefficients, for any given reactor loop configuration.

A computer program which, if adapted to the study of the natural convection problem, would yield detailed information concerning the fluid behavior, is the MAC (Marker and Cell) method of Harlow et al.¹⁶ This is applicable to viscous and nonviscous flow of incompressible fluids, either confined or with a free surface. Presently restricted to two-dimensional cartesian coordinates and problems neglecting thermal effects, it is being modified to consider two-dimensional cylindrical coordinates, heat transfer, and thermal convection. Figures 3 and 4 illustrate some typical results obtained with MAC. Figure 3 has no connection with reactor safety problems, but is an impressive demonstration of the code's ability to treat fluid flow problems with a free surface. It illustrates the behavior of fluid striking an obstacle following a dam rupture. Figure 4 shows the results of calculations performed on a confined fluid; starting with a high density fluid atop a low density fluid, a sine-wave disturbance is impressed on the interface.

C. Integrated Reactor Analysis

Transient analysis of an entire fast reactor plant is of importance both for studies of plant and reactor safety and for application to design of plant components. Thus, for example, the reactor core behavior following a load demand cannot be determined with an analysis

Fig. 3. Water from a Reservoir (From Ref. 16)

The dam holding the reservoir is removed at $t = 0$. Subsequently, the water falls away toward the obstacle in its path. The collision and splash over the top of the obstacle are shown in the last two frames. The calculated pressure history on the obstacle can then be used to predict damage. The bottom allows free slip, and the viscosity is negligible. Comparison of similar calculations (but lacking an obstacle) have been made with the results of experiments, and the agreement is well within experimental error.

Fig. 4. Instability of a High Density Fluid Above a Low Density Fluid. (From Ref. 16)

which treats only the reactor core since the entire plant--from core to heat dump--affects core response to a load demand. Figures 5 through 10 show the results of calculations performed with one version of the RAPID (Reactor and Plant Integrated Dynamics) code.¹⁷ The curves describe some of the results of calculations performed for the Molten Plutonium Burnup Experiment (MPBE) in the Fast Reactor Core Test Facility (FRCTF). With the reactor initially critical at 20 kW, an instantaneous increase of power demand from 20 kW to 20 MW was assumed to have been imposed. Primary and secondary coolant flow rates were maintained at their normal full power values, and control rods were not moved during the calculation.

This RAPID code presently employs the point neutron kinetics equations (modified to avoid the aforementioned problems caused by small prompt neutron generation time) coupled with heat transfer and flow equations, all solved by standard finite difference techniques. It considers reactor, vessel, piping, heat exchangers, heat dump, primary and secondary loops, reactivity feedback, coolant transport time, any core size, any (variable) power level, fission product decay heating, any coolant flow rates, any realistic plant perturbations, and arbitrary mass, area, volume and material for each component in the plant. The changes planned for RAPID in the immediate future are: replacing the existing neutron kinetics solution by Vigil's continuous analytic continuation treatment; replacing the finite difference core heat transfer calculations by Axford's analytic solution; adding a steam cycle subroutine, complete with preheater, boiler, superheater, turbine, condenser, pipes and valves; and adding several primary and secondary sodium loops.

III. GENERAL

All of the working codes mentioned above have been programmed for either the IBM-7094 or the IBM-7030 computers, most for the former. With the installation of the CDC-6600 at LASL (roughly 20 times faster than the 7094 and with core storage initially twice and

Fig. 5. MPBE Core and Heat Dump Power vs Time.

Fig. 6. MPBE System Flow Rates vs Time.

Fig. 7. MPBE Heat Dump Temperatures vs Time.

Fig. 8. MPBE Heat Exchanger Temperature vs Time.

Fig. 9. MPBE Core Temperatures vs Time.

Fig. 10. MPBE Core Excess Reactivity vs Time.

ultimately four times as large as the 7094) marked improvement of the codes is possible, both from the standpoint of accuracy and calculational speed. All of the figures shown are direct computer output from the SC-4020 film plotter.

REFERENCES

1. Okrent, D., J. M. Cook, D. Satkus, R. B. Lazarus, and M. B. Wells, "AX-1, A Computing Program for Coupled Neutronic-Hydrodynamics Calculations on the IBM-704," ANL-5977 (1959).
2. Chezem, C. G., and W. R. Stratton, "RAC--A Computer Program for Reactor Accident Calculations," LAMS-2920 (1963).
3. Peterson, D. M., Private communication (1966).
4. Carmichael, B. M., Private communication (1966).
5. Hannum, W. H., and B. M. Carmichael, "DPC--A Two-Dimensional Data Preparation Code," LA-3427-MS (1965).
6. R. B. Nicholson, "Methods for Determining the Energy Release in Hypothetical Fast Reactor Meltdown Accidents," NSE 18, 207 (1964).
7. Wolfe, B., N. Friedman, and D. Riley, "Influence of Doppler Effect on the Meltdown Accident," ANL-7120, p. 171 (1963).
8. Meyer, R. A., and B. E. Wolfe, "High Temperature Equation of State of Uranium Dioxide," ANS Trans. 7, 1 (1964).
9. Menzies, D. C., "The Equation of State of Uranium Dioxide at High Temperature and Pressures," TRG-Report-1119 (1966).
10. Deal, W. E., "Dynamic High Pressure Techniques," in Modern Very High Pressure Techniques, R. H. Wentorf, Ed., Butterworths, Washington (1962).
11. Vigil, J. C., "Solution of the Nonlinear Reactor Kinetics Equations by Continuous Analytic Continuation," LA-3518 (1966).
12. Lathrop, K. D., Private communication (1966).
13. Axford, R., Unpublished notes (1966).
14. Greebler, P., D. B. Sherer, and N. H. Walton, "FORE--A Computational Program for the Analysis of Fast Reactor Excursions," GEAP-4090 (1962).
15. Goplen, B. C., and J. D. Cleary, Private communication (1966).
16. Welch, J. E., F. H. Harlow, J. P. Shannon, and B. J. Daly, "The MAC Method--A Computing Technique for Solving Viscous, Incompressible, Transient Fluid-Flow Problems Involving Free Surfaces," LA-3425 (1965).
17. Anderson, C. A., Unpublished notes (1966).