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SUMMARY OF COMPUTER CODES
USED FOR FFTF CONTAINMENT
AND SITING STUDIES

FEBRUARY 1971

HANFORD ENGINEERING DEVELOPMENT LABORATORY
UNITED STATES ATOMIC ENERGY COMMISSION

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Compiled
by

Staff of Safety and Systems Analysis Engineering

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SUMMARY OF COMPUTER CODES USED FOR FFTF CONTAINMENT AND SITING STUDIES

INTRODUCTION

Containment and siting studies for the Fast Flux Test Facilities were conducted to assure adequate margins for public protection against unforeseen events. These studies consisted of analyses of postulated events of an extreme nature beyond any realistic probability for occurrence. Consequences were then investigated analytically to assess the design margins against such unlikely events. Because of the complex nature of these analytical models, it was necessary to use computer codes for these evaluations. The scope of these codes covers the initiation of a hypothetical accident, its immediate consequences in terms of energy, pressure and temperature effects and long term consequences involving the potential for leakage of radioisotopes from containment to the environs and the potential dose at the site boundary.

Because the codes utilized in these assessments are in various stages of documentation, it is desirable to provide a summary description of each. The codes used in each area of analysis are as follows:

	<u>Codes Used</u>	<u>Originator</u>
• Initiating Mechanisms, Core Disruption and Disassembly	FREADM-1 SAS1A MELT-II VENUS	GE ANL HEDL ANL
• Work Energy	SOCOOL-II	HEDL
• Mechanical Effects on Core Structures	ASPRIN REXCO-H	HEDL ANL
• Pressures and Temperatures from Sodium Spills	SOFIRE-II CACECO	AI HEDL
• Radiological Effects	ISOSHL INDOSE II EXDOSE RIBD COMRADEX HAA-3A	HEDL HEDL HEDL HEDL AI AI

These codes form a relatively complete series of analytical models that may be used to evaluate consequences at any stage of postulated accidents of a severe type.

In the summaries which follow, a brief description of complexities, uncertainties and experimental verification, if any, is given. Other information of interest includes method of analysis and items related to use of the codes.

ASPRIN⁽¹⁾

1. Name of Code: ASPRIN. Originator: HEDL.
2. Computer for which Program is Designed: UNIVAC 1108.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: This code programs a simplified method for calculating the vessel response to a core disruptive accident and determines loadings on the vessel cover and subsequent containment barriers. ASPRIN serves as a short running time design tool for investigating effects of reactor design changes and requirements.
4. Method of Solution: Maximum cover loadings are assumed to result from a coolant slug propelled against the cover by inertial pressures in the core region. The analytical model for predicting these head loadings and vessel responses utilizes combinations of 1-dimensional Newtonian models in radial and axial directions to simulate the reactor, cover, and holddown structure. Wave phenomena are not considered and deformations are assumed to occur from quasi-steady pressures. The vessel support structure is modeled as elastic-plastic with linear strain hardening.

Output information consists of gross vessel and cover displacements, velocities, stresses, strains, and the energy distribution.
5. Restrictions on the Complexity of the Problem and Uncertainties: The analytical model consists of a gaseous bubble in the core region acting upon and moving the surrounding structures and the coolant slug. Their movement is considered primarily by Newtonian type mechanisms rather than by compressible wave action.

Application of the model thus is limited to time periods greater than several wave reflections and pressure regimes where the coolant compresses less than 2 or 3%. Material laws are considered in the structures resistance to motion.

Also, each simulated structure is modeled as a single point.

The head loadings are probably not precise, but they are conservatively high.

6. Related and Auxiliary Programs: The numerical integrations of the differential equation is by an Adams-Moulton variable step, predictor corrector method included in the UNIVAC 1107 BEEF MATH ROUTINES.⁽²⁾
7. Running Time: A typical problem runs about 60 seconds on the UNIVAC 1108.
8. Unusual Features: The code is designed primarily for scoping studies on slug energy dissipation in the reactor head area.
9. Status: A production code is available from WADCO, Hanford Engineering Development Laboratories.
10. Machine Requirements: 7k of core storage is adequate.
11. Experimental Verification: In order to verify the conservatism of the analytical model, the predicted results of the SL-1 accident have been compared to available measured data. It is important to note that ASPRIN, as it is conventionally used, underpredicted the vessel radial deformation and over-predicted the kinetic energy remaining in the coolant slug and cover system. Hence, the analytical model overpredicts the cover loadings which might occur as the result of a core disassembly accident.
12. References:
 1. G. L. Fox. ASPRIN - A Computer Code for Predicting Reactor Vessel Response to Hypothetical Maximum Accidents on Fast Reactors, BNWL-1166, December 1969.
 2. UNIVAC 1107 BEEF MATH ROUTINE. Share write-up RWDE2F, Section D2.

CACECO

1. Name of Code: CACECO. Originator: HEDL
2. Computer for which Program is Designed: UNIVAC 1108.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: The CACECO code predicts the pressure and temperature histories of 1, 2, 3, or 4 containment spaces of a sodium cooled reactor which may be involved in a loss of sodium accident. Each containment space (e.g., reactor cavity, pipeway, equipment cell, or reactor building) has an atmosphere and may have a sodium pool. The atmosphere consists of nitrogen, oxygen, sodium vapor, and decay heat fission products. The atmosphere is assumed to be well mixed and is characterized by a uniform temperature and composition. The sodium pool, if it exists, is also well mixed and is characterized by a uniform temperature which is usually different from the atmosphere temperature. The roof, walls, floor, and equipment of each containment space are represented by one or more heat conducting structures whose thermal behaviors can be described by one-dimensional, multi-layer, transient heat conduction equations. The histories of sodium vapor injection into any atmosphere, of sodium liquid spray into any atmosphere, of nitrogen-oxygen mixture injection into any atmosphere, and of sodium liquid spill into any pool are assumed available from previous calculations and are the input data that defines the accident for the CACECO code. The code calculates the energy additions due to decay heating in any atmosphere or pool, energy reductions due to space coolers in any containment space, and the atmosphere vent and leakage flows between any of the containment spaces or

to the outside. The code also calculates the effects of sodium vapor-oxygen reaction in any atmosphere, of sodium liquid spray-oxygen reaction or spray evaporation and heating of any atmosphere, of sodium condensation out of any atmosphere, of sodium-oxygen reaction or sodium evaporation at the surface of any pool, and the boiloff of any sodium pool into the atmosphere of the containment space. The code output includes the atmosphere temperature and weight in each containment space, the vent and leakage flow rates and integrated flows between containment spaces and to the outside, the heat transfer rates and integrated heat transfers at the surfaces of all heat structures, and the temperature distributions through all of the heat structures.

4. Method of Solution: The initial weight composition of the atmosphere of each containment space is calculated from input data and the initial temperature distributions through all of the heat structures are calculated from the steady state solution of the heat conduction equations. The differential equations are solved by a predictor-corrector marching calculation. A time advancement proceeds as follows.

The decay heating of the assigned atmospheres and pools is evaluated at the midpoint of the time interval. The sodium vapor and liquid additions rates and the nitrogen and oxygen addition rates are evaluated at the midpoint of the time interval and, with attendant energies, are added to the atmosphere or pool of the assigned containment space. The heat removed by the space coolers over the time interval is evaluated and subtracted from the atmosphere energy of the assigned space. The sodium-oxygen reaction rate or sodium evaporation rate at the surface of each sodium pool is evaluated based on the atmosphere and pool surface conditions at the beginning of the time interval and

the attendant material and energy effects over the whole interval are added to the atmosphere and pool. The atmosphere vent flow rates and leakage rates between containment spaces and to the outside are evaluated based on atmosphere conditions at the beginning of the time interval and the attendant material and energy effects over the whole interval are added to the atmospheres. Heat transfer rates between the heat structures and the atmosphere and pool of each containment space are summed at the beginning of the time interval and the attendant energy effects over the whole interval are added to the atmospheres and pools. Atmosphere temperature and pressure and pool temperature in each containment space at the end of the time interval are predicted by solving appropriate material, energy, and volume balance equations. Using these results as boundary conditions, the heat conduction equations are advanced over the time interval using an implicit calculation technique. The resulting heat transfer rates at the end of the time interval are summed to correct the previous estimates of energy effects into the atmospheres and pools. Also, the atmosphere vent flow rates and leakage rates are re-evaluated using predicted conditions at the end of the time interval and the attendant material and energy effects are used to correct the previous effects. The corrected atmosphere temperature and pressure and pool temperature in each containment space are found by solving the material, energy, and volume balance equations a second time.

5. Restrictions on the Complexity of the Problem:
Atmosphere and pool temperatures should be in the range of 50 °F to 2500 °F due to limits of accurate thermodynamic properties for superheated sodium vapor and saturated sodium vapor and

liquid. The core storage assigned heat structure data restricts the number of heat structures to less than 96. Further, the trade-off between the number of heat structures and the maximum number of mesh points in any structure is defined by the following equation:

$$\text{Storage} = 121 N + 8 N^2 + 5 M (1 + N) < 20,000$$

where: N is the number of heat structures and
 M is the number of mesh points per structure.

For example, a feasible number of structures is about 40 when at least one structure has 35 mesh points. Finally, the heat structures are limited to 20 different materials of constant thermal conductivity and heat capacity. Heat transfer coefficients may depend upon time, average film temperature, or temperature difference but are usually taken as natural convection coefficients. These coefficients may be enhanced by the local condensation of sodium vapor. Radiation heat transfer is based upon the assumption of grey surfaces having constant values of area, geometrical view factor, and emissivity. The atmosphere may range from opaque to transparent to thermal radiation. Atmosphere vent and leakage flow rates are based upon pressure differences and will not account for natural convection flows between vertical containment spaces, the lower space having a higher temperature than the upper space.

6. Uncertainties with Program Usage: The two types of uncertainties associated with the CACECO code are: (A) the mathematical equations that model natural phenomena and (B) the input data that model containment facilities. Examples of the uncertainties due to the equations are given below:
 - a. Discrete values are used to represent continuous distributions. For example, the calculated atmosphere temperature of a containment space is a discrete value whereas the cavity, cell,

or pipeway modeled by the containment space would have a distribution of atmosphere temperatures, higher near heat sources and lower near heat sinks, because of natural convection. For another example, the calculated temperatures of a heat structure vary through the depth of the structure whereas roof, wall, floor, or equipment component modeled by the heat structure would have a distribution of surface and material temperatures because of variation of convection and radiation over the surfaces and conduction throughout the material.

- b. A step change in the atmosphere or pool temperature, particularly when associated with heat transfer coefficients greater than about $250 \text{ Btu/hr-ft}^2\text{-}^\circ\text{F}$, or a step increase in the volumetric heat generation within a heat structure will initiate oscillations, which damp to zero, in the surface and near surface temperatures of the affected heat structures.
- c. The heat and mass transfer rates calculated by the POOLR subroutine to represent the sodium-oxygen reaction at the surface of a sodium pool and the effective heat transfer coefficients calculated by the Colburn and Hougen method⁽²⁾ to represent natural convection heat transfer and local condensation of sodium vapor on the roofs, walls, and equipment must be increased by a factor of 2 (approximately) to agree with the rates calculated by the SOFIRE-II code.
- d. The heat and mass transfer rates calculated by the RXRATE subroutine to represent the sodium-oxygen reaction at the surface of a sodium spray particle go to zero, and then

to negative values, as the atmosphere temperature approaches the vapor phase reaction temperature, and then exceeds the latter.

Examples of the uncertainties due to the input data are given below.

- a. The vessel rupture, pipe break, or other accident must be described in terms of material and energy transfers into the containment spaces, volumetric heat generation within the heat structures, heat transfer conditions at the surfaces of the heat structures, and effectiveness of the atmospheric space coolers. These terms mean that the accident and resulting conditions have to be defined at the outset, by other methods, or by iteration through a succession of CACECO problems.
- b. The facility and equipment must be described in terms of containment spaces, vent areas and/or leakage rates between these spaces and to the outside, heat structures, temperature histories for heat sources and sinks, and atmospheric space cooler capacities. These terms mean that there must be engineering data and/or drawings on all pertinent features of the facility and equipment. An example of uncertainty is the decision as to which features are pertinent to the problem.
- c. The various ways to model the roofs, walls, floors, and equipment as one-dimensional, slab, cylindrical, or spherical heat structures pose uncertainties which are amenable to analysis. For example, the CACECO code could provide histories, following an accident, of various boundary conditions for a detailed analysis of any structure or component by a two or three dimensional heat conduction code. For another example, the CACECO code provides the temperature, heat

transfer rate, and integrated heat transfer data for checking such items as the following:

- 1) Various distributions of mesh point spacing on the accuracy of heat conduction calculations;
- 2) Importance of sideway conduction, which is not treated by the CACECO code; for example, a 40 ft high wall could be successively modeled as two 20 ft high walls, four 10 ft high walls, and eight 5 ft high walls to approach the temperature variation over the height of the wall;
- 3) Relative importance of conduction or convection versus radiation heat transfer at the surfaces of various structures through successive periods of the accident history; for example, the facility design that uses a sheet steel liner to cover the concrete walls of a sodium equipment cell may be modeled, depending upon the thickness of the gap (due to concrete shrinkage and steel expansion) between the steel and concrete surfaces as:
 - (a) one heat structure with heat conduction across the gas gap or
 - (b) two structures, one for the steel and the second for the concrete, with conduction or convection and radiation heat transfer across the gas gap;
- 4) Importance of zoning the surfaces of the various structures when radiation heat transfer is more important than convection heat transfer; for example, in an analysis of a spill of hot sodium, the reactor vessel, the steel lined concrete roof, walls, and floor of the reactor cavity, and the sodium pool (itself, a heat structure)

could be modeled with successively more zones (levels) of vessel and wall to better account for the distribution of radiant energy from the sodium pool on the floor. In this example, one to five levels of vessel and wall could be checked in succession by changing the input data listed below.

<u>Number of Levels of Vessel and Walls</u>	<u>Number of Radiation Zones</u>	<u>Described Number of Heat Structures (input data)</u>	<u>Number of Radiation Area-View-Emissivity Factors (input data)</u>
1	10	8	13
2	14	11	25
3	18	14	41
4	22	17	61
5	26	20	85

Six levels of reactor vessel and cavity wall would require radiation area-view-emissivity factors that would exceed the present CACECO code storage limit of 95 factors.

- d. The uncertainties with CACECO code analysis are reduced by devoting the maximum available time to the description of the heat structures.
7. Related and Auxiliary Programs: The CACECO code was developed for sodium cooled reactors from the CONTEMPT code⁽¹⁾ which was developed for water cooled reactors. The MASTER program provides special access to the material properties and temperatures of the heat structures. The NAPROP subroutine provides thermodynamic properties for sodium.⁽³⁾ The SRCHP and SRCHUL subroutines provide the temperature at a given sodium vapor pressure and liquid energy, respectively. The POOLR subroutine calculates the burning evaporation rate at the surface of a sodium pool.⁽⁴⁾ The RXRATE subroutine calculates the burning-evaporation rate of a single particle of sodium spray.⁽⁵⁾ The TIMEDP subroutine provides logarithmic interpolation of decay power data. The TABLU and TABLG subroutines

provide linear interpolation of data tables. The INPUT subroutine checks the input data for consistency and sufficiency and calculates constant parameters of the heat conduction equations. The CVIRDP subroutine reads input data cards having a rigid or relaxed format. The few system subroutines used are for date, time of day, computer running time, and divide check.

8. Running Time: The heat structure calculations take 50% to 70% of the running time of the typical problem. An average problem with 10 heat structures and a total of 203 mesh points takes about 0.072 seconds per time interval step of the marching calculation. A problem with no vent flows between containment spaces can run with about 33 time intervals per problem hour. A problem with vent flows between containment spaces will run with 300 to 3,000 time intervals per problem hour.
9. Unusual Features: The CACECO code has restart capability. All of the required data at the end of the scheduled problem or at 10 seconds before the end of the assigned computer running time is written onto tape. This tape can be read later to restart the problem at the next time interval. The code also has the capability to vary the time interval of the marching calculation. The criterion used to vary the time interval is the sum of the differences between predicted and corrected atmosphere energies of the 1 to 4 containment spaces. A sum amounting to less than 0.001% of the energies will double the size of the next time interval while a sum greater than 0.1% will halve the next interval. This criterion is nearly equivalent to doubling the next interval when the predicted temperatures are within 0.005% of the

corrected temperatures and halving the next interval when the predicted temperatures differ by more than 0.5% from the corrected temperatures.

Vent flow rates between containment spaces and to the outside are calculated using the standard nozzle equation for compressible gas flow for both subsonic and sonic flow rates. Vent flow is assumed when the vent area is given in the input data. In contrast, leakage flow between spaces and to the outside is assumed when the input data are leakage rates at a given density and pressure difference.

10. Status: The CACECO code is in production. It has not been distributed outside of WADCO.
11. Machine Requirements: 53K of core memory is adequate.
12. Other Programming or Operating Information or Restrictions: None.
13. Verification: The CACECO code has been checked against the SOFIRE-II code by using identical problems. SOFIRE-II, in turn, has been shown to compare favorably with experimental pool fire data.⁽⁴⁾

14. References:

1. L. C. Richardson, L. J. Finnegan, R. J. Wagner, and J. M. Waage. CONTEMPT, A Computer Program for Predicting the Containment Pressure-Temperature Response to a Loss-of-Coolant Accident, IDO-17220, Phillips Petroleum Company, June 1967. Note, the code is available from the Argonne Code Center, and is described as Code Abstract 297 by M. K. Butler, Marianne Legan, and L. Ranzini, Argonne Code Center: Compilation of Program Abstracts, ANL-7411, Supplement 1, p 450, October 1968.
2. A. P. Colburn and O. A. Hougen. Ind. and Eng. Chem., 22, 522, 1934.

3. G. H. Golden and J. V. Tokar. Thermophysical Properties of Sodium, ANL-7323, August 1967.
4. R. P. Johnson, M. Silberberg, J. Hopenfeld, and P. Bureger. "Characterization of Sodium Pool Fires", pp 195-205, Proceedings of the International Conference on Sodium Technology and Large Fast Reactor Design, November 7-9, 1968, ANL-7520, Part 1.
5. Theresa S. Krolikowski. Violently Sprayed Sodium-Air Reaction in an Enclosed Volume, ANL-7472, September 1968.

COMRADEX⁽¹⁾

1. Name of Code: COMRADEX. Originator: AI.
2. Computer for which Program is Designed: The program can be run on the UNIVAC 1108, IBM System/360 Mod 50, and the SC-4020.
Programming Language: Fortran V.
3. Nature of the Physical Problem Solved: COMRADEX calculates the radiation dose resulting from the direct gamma dose potential from the building, the internal dose caused by inhalation of activity in the released cloud, and the external gamma dose from immersion in the cloud.
4. Method of Solution: COMRADEX requires as input an inventory, parameters describing the release to the atmosphere, and times and distances of interest. COMRADEX then calculates the activity released to the atmosphere, accounting for leakage from and cleanup processes within up to four barriers of containment. Dispersion of the released plume is calculated after the model of Pasquill.^(2,3) COMRADEX then calculates the internal and external doses associated with the cloud and the external doses associated with radioactivity in the building at the downwind points and times of interest.
5. Restrictions on the Complexity of the Problem and Uncertainties: COMRADEX is not equipped to evaluate depletion of the cloud by fallout, rainout, or washout or to calculate the doses which would result from the deposited activity. The shielding afforded by air between the building and the downwind points of interest is calculated by COMRADEX by assuming attenuation and buildup factors appropriate to 3-MeV photons. Perfect reflection of the cloud at the ground surface is also assumed. Internal doses are based on the standard ICRP methods⁽⁴⁾; the new lung model⁽⁵⁾ is not used.

6. Related and Auxiliary Programs: COMRADEX is programmed to accept output cards from the inventory code CURIE.⁽⁶⁾ The subroutine CONVL solves the multiple containment equation by a numerical method developed by E. R. Cohen.
7. Running Time: Machine times of 200 to 400 seconds are typical for problems analyzed with COMRADEX.
8. Unusual Features: COMRADEX permits evaluation of the effects of fallout within each containment device. These cleanup factors may be varied during the time of interest. Up to four-barrier containment may be evaluated. The calculation of external dose from exposure to the cloud is for a finite cloud in COMRADEX. COMRADEX also calculates the external dose resulting from exposure at various downwind distances to the radioactivity remaining in the building.
9. Status: The object deck of COMRADEX, W00088, is on file at Atomics International.
10. Machine Requirements: Requires 131K UNIVAC 1108.
11. Other Programming or Operating Information or Restrictions: Cards punched in BCD.
12. Experimental Verification: Code has not been verified in total but formulations used in the model are by integral experiments based on established experimental data.
13. References:
 1. G. W. Spangler, M. Boling, W. A. Rhoades, and C. A. Willis. "Description of the COMRADEX Code", AI-67-TDR No. 108, August 1, 1967.
 2. F. Pasquill. Atmospheric Diffusion, D. Van Nostrand Co., Ltd., 1962.
 3. W. F. Hilsmeier and F. A. Gifford, Jr. "Graphs for Estimating Atmospheric Dispersion", ORD-545, July 1962.

4. International Commission on Radiological Protection, Report of Committee II on Permissible Dose for Internal Radiation, ICRP Publication 2, Pergamon Press, New York, N. Y., 1959.
5. Task Group on Lung Dynamics. "Deposition and Retention Models for Internal Dosimetry of the Human Respiratory Tract, Health Physics, Vol. 12, pp 173-207, February 1966.
6. G. P. Kenfield, W. R. Lahs, W. B. Sayer, R. M. MacAdams, and N. A. Harris. "Curie-Dose-Thunderhead - A Digital Computer Program for External and Internal Radiation Dose Calculations", NAA-SR-8884, June 15, 1965.

EXDOSE⁽¹⁾

1. Name of Code: EXDOSE. Originator: HEDL
2. Computer for which Program is Designed: The program can be run on the UNIVAC 1108 and IBM 7090.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: EXDOSE calculates the external gamma radiation dose to the total body resulting from immersion in a half-infinite cloud of fission products.
4. Method of Solution: EXDOSE requires as input the amount of fuel involved, the duration and conditions of the irradiation, the atmospheric conditions, and the distance to the point of interest. EXDOSE then calculates the fission product inventories by means of a modified RIBD⁽²⁾ subroutine (if non-fission product activities are investigated, RIBD is not used and the inventory of the radionuclide(s) of interest must be entered as input data), amount of activity released, dispersion of the plume by the Sutton^(3,4) or Simpson-Fuquay⁽⁵⁾ equations, and the dose at the specified downwind point.
5. Restrictions on the Complexity of the Problem and Uncertainties: EXDOSE assumes that the individual is immersed in a cloud of half-infinite extent that is at a uniform concentration equal to that at the point of interest. The calculation also assumes perfect plume reflection at the ground surface. EXDOSE is not equipped to handle fallout within containment nor the effects on downwind radiation exposure of multibarrier containment. While EXDOSE does permit reduction of downwind cloud concentration by accounting for deposition from the cloud, doses due to this fallout are not calculated by EXDOSE.

6. Related and Auxiliary Programs: EXDOSE includes RIBD as a subroutine to permit calculation of source strength from known fuel inventory and irradiation history. RIBD has been modified for EXDOSE to include, 1) release of fission products at an exponential rate and, 2) arbitrary factors at up to two decay times to account for only partial release of fission products from fuel and to account for filtration.
7. Running Time: Computer time is nominal if cloud depletion is not included. Requirements are about 5 seconds per group of 50 (E/q) calculations if the Simpson-Fuquay equations are used and about 5 seconds per group of 10 (E/q) calculations if Sutton's equations are used.
8. Unusual Features: EXDOSE calculates a source that consists of fission products by the subroutine RIBD. The source may then be released at an exponential rate to account for the effects of a single containment. Cloud depletion by fallout during dispersion can be calculated by EXDOSE.
9. Status: The program is being expanded to permit greater flexibility in the problems handled.
10. Machine Requirements: Requires 131K UNIVAC 1108.
11. Other Programming or Operating Information or Restrictions: Cards punched in BCD.
12. Experimental Verification: No integral experiment verification but formulations used in the model are based on experimental data.
13. References:
 1. M. M. Hendrickson. "EXDOSE - A Computer Program for Calculating the External Gamma Dose from Airborne Fission Products", BNWL-811, September 1968.

2. R. O. Gumprecht. "Mathematical Basis of Computer Code RIBD", DUN-4136, June 17, 1968.
3. O. G. Sutton. Micrometeorology, McGraw-Hill Book Company, New York, N. Y., 1953.
4. D. H. Slade, Ed. "Meteorology and Atomic Energy 1968", TID-24190, July 1968.
5. J. J. Fuquay, C. L. Simpson, and W. T. Kinds. "Estimates of Ground Level Air Exposures Resulting from Protracted Emissions from 70 Meter Stacks at Hanford", HW-80204, 1964.

*FREADM-1⁽¹⁾

1. Name of Code: FREADM-1. Originator: GE
2. Computer for which Program is designed: GE635.
Programming Language: Fortran IV.
3. Nature of Physical Problem Solved: FREADM-1 is a fast reactor multi-channel accident analysis program designed to efficiently simulate a reactor transient from initiation to the point of core disassembly. Models are included for nuclear kinetics (point model), core thermo-hydraulics, voiding, fuel redistribution, failure propagation, programmed reactivity insertion, and the dynamics of primary system coolant flow. A broad range of assumed accident initiating and propagating activities may be simulated using triggering logic included in the code. FREADM-1 is restricted to accidents which initiate and propagate uniformly within annular or cylindrical coaxial core regions.
4. Method of Solution: Time integration of the equations for the dynamics of nuclear kinetics, heat transfer and primary loop coolant flow may be performed in a coupled mode, or independently. Transient temperature conditions computed for single pins, representative of a number of bundle types, may be used to initiate prescribed accident initiating and/or propagating activities. The user supplies criteria for initiating these activities. Reactivity feedback from the various activities may be computed using models in the code, or input from tables.
5. Restrictions on the Complexity of the Problem and Uncertainties: Heat transfer calculations for up to 12 radial core regions may be performed simultaneously with up to 12 separate bundle types subdivided into 9 or less axial sections. Radial heat transfer

*FREADM has not been used directly in FFTF accident analyses to date, but is being used in conjunction with safety development programs involving fuel failure phenomena of applicability to FFTF.

calculations are done using up to 10 radial fuel nodes, a clad node and a coolant node for each axial section. Loop flow may be treated using a maximum of 2 independent primary coolant loops (loops may be of different size to simulate more than 2 loops). Point kinetics with up to 6 delayed neutron precursor groups is used to compute the transient power level of the core.

A point kinetics formulation is used which is probably non-conservative. It is suspected, however, that significantly large uncertainties are inherent in the present models for molten fuel motion and coolant expulsion. No coolant re-entry model is included in the present version. Detailed loading on the cladding cannot be done because only one fuel material type is treated and fuel expansion, due to density reduction or fission gas release, is not taken into account. (A later version, however, is anticipated to include the TOFF, transient overpower fuel failure, routine to estimate the effects of fission gas release). A natural source of pin failure incoherency, due to statistical fluctuations and differing power ratings in the subassemblies and rings of subassemblies, is ignored.

6. Related and Auxiliary Programs: The coolant voiding sub-routine, VOIDUM, is coupled directly to the FREADM-1 package but may be run independently for exploring the characteristics of the primary system coolant dynamics separately in a tank or pot type sodium cooled reactor.
7. Typical Running Time: Running time for FREADM-1 is strongly dependent on the running option used and values supplied for time step control. Sample problems which have been run indicate the following breakdown:

- a) 200 kinetics time steps with Doppler feedback for 12 bundle types, 9 axial sections used $\sim 1.5/100$ hrs of GE-635 processor time.
 - b) 87 coupled kinetics and heat transfer time steps using 12 bundle types and 9 axial sections used 7.3/100 hrs of GE-635 processor time.
 - c) 32 coupled loop flow, kinetics and heat transfer time steps using 12 bundle types and 9 axial sections used 7.7/100 hrs of GE-635 processor time.
8. Unusual Features of the Program: FREADM-1 is highly flexible both in the complexity of the problem solved and the selection of solution methods. Loop flow, kinetics and heat transfer calculations may be done separately or in a coupled mode. Trigger logic provided in FREADM-1 permits the sequence of accident initiating and propagating activities to be determined based on computed local conditions reaching preset levels input by the user. Tables are available which permit a flexible description of the processes for parametric studies. By controlling the time step size in the kinetics calculation, time steps for heat transfer and loop flow calculations are performed with time steps determined by accuracy requirements on these processes only. An integral number of kinetics steps may be taken per heat transfer step. Input to the code is in free form with much input which is optional.
9. Status: Production.
10. Machine Requirements: Computer memory -- 24K. Peripheral storage units - 3.
11. Experimental Verification: None.
12. References:
1. D. D. Freeman, et al. "The FREADM-1 Code - A Fast Reactor Excursion and Accident Dynamics Model", June 1970, (GEAP-13608).

HAA-3A^(1,2)

1. Name of Code: HAA-3A. Originator: AI.
2. Computer for which Program is Designed: The program can be run on the UNIVAC 1108 and the IBM System/360 Mod 65.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: HAA-3A calculates the agglomeration, settling, wall plating, and leakage of a heterogeneous aerosol as a function of time.
4. Method of Solution: HAA-3A requires as input information regarding the aerosol behavioral processes to evaluate, the times involved, and physical data on the space into which the aerosol is introduced. HAA-3A then calculates the time-dependent masses for plated, settled, suspended, and leaked material. The program evaluates an approximation to the general integro-differential equation which describes the behavior of an aerosol.⁽³⁾ The approximation is the requirement that the size distribution function be log-normal. When the agglomeration process becomes negligible, the aerosol distribution does not remain log-normal. HAA-3A therefore ignores agglomeration at this point, and subsequent aerosol behavior is calculated by a stirred settling model. HAA-3A also accounts for changes in settling velocity with particle size by incorporating the empirical Klyachko velocity correction⁽⁴⁾ to describe the departure from Stokes' Law.
5. Restrictions on the Complexity of the Problem: HAA-3A described aerosol behavior in one containment, only. Output for a case must be entered as the source term for the next containment, and the program must be run again.

6. Related and Auxiliary Programs: HAA-3A contains the subroutine SSM which describes the behavior of an aerosol that is settling and leaking but is not agglomerating or plating. HAA-3A output can be used as input to HAA-2⁽⁵⁾ which evaluates by numerical integration the general integro-differential which describes aerosol behavior. HAA-2 is used for aerosol mass concentrations of less than 4 $\mu\text{g/cc}$.
7. Running Time: Typical running time is about 30 seconds per case on the IBM System/360 Mod 65.
8. Unusual Features: HAA-3A uses a stirred settling model when the aerosol concentration becomes small and the Klyachko velocity correction for large particles and large settling velocities. The program also includes a correction for non-Stokesian shape.⁽⁶⁾ Time-dependent plating constant, source rate, and leakage rate may be used.
9. Status: The object deck of HAA-3A, W50140, is on file at Atomics International.
10. Machine Requirements: Requires 131K UNIVAC 1108.
11. Other Programming or Operating Information or Restrictions: Cards punched in BCD.
12. Experimental Verification: Code is composed of experimentally verified models for agglomeration and settling. Prediction of small-scale experiments has been successful.
13. References:
 1. R. S. Hubner. "Program HAA-3A: A Modification of the Computer Program HAA-3", TI-707-13-003, May 1970.
 2. R. S. Hubner. "An Approximate Solution to the General Equation for the Coagulation of Heterogeneous Aerosols", AI-AEC-MEMO-12880, September 26, 1969.

3. M. A. Greenfield, R. L. Koontz, and D. F. Hausknecht.
"Characteristics of Aerosols Produced by Sodium Fires.
Vol. II. Comparisons of Experiment with a General
Equation for the Coagulation of Heterogeneous Aerosols",
AI-AEC-12878, October 31, 1969.
4. N. A. Fuchs. The Mechanics of Aerosols, Pergamon Press,
New York, N. Y., 1964.
5. D. F. Hausknecht. "User's Manual for the Aerosol
Agglomeration Code, HAA-2", AI-TDR-12743, September 25, 1968.
6. R. L. Koontz, et al. "Aerosol Modeling of Hypothetical
LMFBR Accidents", AI-AEC-21977, August 1970.

INDOSE II

1. Name of Code: INDOSE II. Originator: HEDL.
2. Computer for which Program is Designed: The program can be run on the UNIVAC 1108.
Programming Language: Fortran V.
3. Nature of the Physical Problem Solved: INDOSE II calculates the internal radiation doses from inhalation and ingestion of fission products.
4. Method of Solution: INDOSE II requires as input a radionuclide inventory, parameters describing the release to the atmosphere, atmospheric conditions, distances and times for which dose calculations are of interest, and the organ dose calculations desired. INDOSE II then calculates the material released to the atmosphere, accounting for up to four barriers of containment and aerosol behavior after the model of Koontz, et al.⁽¹⁾
After release INDOSE II calculates plume dispersion by the Sutton^(2,3) or Simpson-Fuquay⁽⁴⁾ equations and the dose at downwind points for specified inhalation/ingestion and retention periods by the methods described by the International Commission on Radiological Protection.^(5,6)
5. Restrictions on the Complexity of the Problem and Uncertainties: INDOSE II handles only fixed-rate fallout within containment. The new lung model⁽⁶⁾ may be used to calculate lung dose, but dose to other organs does not use this lung model. INDOSE II assumed all released materials to be in the respirable range. Because INDOSE II is neither linked with or contains a fission product library, appropriate data for each radionuclide to be examined must be separately entered making use of INDOSE II for more than a few nuclides impractical.

6. Related and Auxiliary Programs: INDOSE II contains a library of physical and biological parameters for over 900 isotope-organ combinations.
7. Running Time: Typically, 10 to 30 seconds of machine time are required for an INDOSE II calculation.
8. Unusual Features: INDOSE II accounts for fallout both within containment and from the diffusing cloud. Up to four-barrier containment may be described by the code. Lung doses may be calculated by the new lung model.
9. Status: The program is in the development stage and has not been published.
10. Machine Requirements: Requires 131K UNIVAC 1108.
11. Other Programming or Operating Information or Restrictions: Cards punched in BCD.
12. Experimental Verification: Not verified by integral experiment but the computer model formulations are based on established experimental data.
13. References:
 1. R. L. Koontz, M. A. Greenfield, D. F. Hausknecht, and M. Silberberg. "Studies of the Distribution of Mass Released into the FFTF Hot Cell after the DBA, Interim Report", AI-68-MEMO-53, May 22, 1968.
 2. O. G. Sutton. Micrometeorology, McGraw-Hill Book Company, New York, N. Y., 1953.
 3. D. H. Slade, Ed. "Meteorology and Atomic Energy 1968", TID-24190, July 1968.
 4. J. J. Fuquay, C. L. Simpson, and W. T. Kinds. "Estimates of Ground Level Air Exposures Resulting from Protracted Emissions from 70 Meter Stacks at Hanford", HW-80204, 1964.

5. International Commission on Radiological Protection, Report of Committee II on Permissible Dose for Internal Radiation, ICRP Publication 2, Pergamon Press, New York, N. Y., 1959.
6. Task Group on Lung Dynamics. "Deposition and Retention Models for Internal Dosimetry of the Human Respiratory Tract", Health Physics, Vol. 12, pp 173-207, February 1966.

ISOSHLD⁽¹⁾

1. Name of Code: ISOSHLD. Originator: HEDL
2. Computer for which Program is Designed: The program can be run on the UNIVAC 1108.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: ISOSHLD calculates gamma ray attenuation for isotope sources in a variety of source and shield configurations.
4. Method of Solution: For most problems ISOSHLD requires as input only the geometry and material composition of the source and the shield(s). ISOSHLD then calculates attenuation by a point kernel integration; for most geometries by Simpson's Rule numerical integration. Buildup factors are calculated by the code based on the number of mean free paths of material between the source and detector points, the effective atomic number of a particular shield region, and the point isotropic NDA buildup data available as Taylor coefficients in the effective atomic number range of 4 to 82.
5. Restrictions on the Complexity of the Problem and Uncertainties: Isotopes that are pure beta emitters and isotopes that yield neutrons by spontaneous fission, (γ, n), or (α, n) reactions are not treated by ISOSHLD. Radionuclides that yield photons of greater than 3 MeV in significant quantities are not handled. Calculations of bremsstrahlung production and attenuation cannot be performed by ISOSHLD.
6. Related and Auxiliary Programs: Source strength in uniform or exponential distribution may be calculated by the linked fission product inventory code RIBD⁽²⁾ or by other options

as desired. Subroutines exist within ISOSHL D that calculate buildup corrections (CONTRL), interpolate calculated buildup factors (BFUNC), and adjust shield thickness to equal the specified source point to dose point distance (ADJUST).

7. Running Time: Running time is dependent on the source geometry selected and increases rapidly as the number of 'kernels' into which the source is divided are increased. Typical running times are 5 to 60 seconds.
8. Unusual Features: ISOSHL D will perform a calculation for a source consisting of a fission product inventory if the linked code RIBD is used. The source examined by ISOSHL D may be distributed exponentially or, in the usual case, distributed uniformly.
9. Status: The program is available through Oak Ridge Radiation Shielding Information Center.
10. Machine Requirements: Requires 131K UNIVAC 1108.
11. Other Programming or Operating Information or Restrictions: Cards punched in BCD.
12. Experimental Verification: None.
13. References:
 1. R. L. Engel, J. Greenborg, and M. M. Hendrickson. "ISOSHL D - A Computer Code for General Purpose Isotope Shielding Analysis", BNWL-236, June 1966.
 2. R. O. Gumprecht. "Mathematical Basis of Computer Code RIBD", DUN-4136, June 17, 1968.

MELT-II

1. Name of Code: MELT-II. Originator: HEDL.
2. Computer for which Program is Designed: UNIVAC 1108.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: MELT-II is a fast reactor multi-channel neutronics-heat transfer accident analysis program designed to efficiently simulate reactor behavior from accident inception to the start of core disassembly. Although a lumped parameter kinetics routine is used, spatially weighted reactivity feedback models include Doppler broadening, fuel redistribution and coolant density decrease and expulsion. Detailed heat-transfer calculations are made for selected fuel pins, each of which is normally assumed to be representative of all pins within a radial ring of subassemblies.
4. Method of Solution: Heat transfer calculations are accomplished by an implicit scheme, removing any geometric constraint on the size of the time step. The efficient method used to solve the kinetics equations is stable for very substantial increases in the power per step. Accuracy is controlled by forcing a recalculation of the temperature, feedback terms, etc. at a reduced time step if the power computed using an extrapolated feedback in the first pass does not agree, within a specified criterion, with the power computed using the actual feedback. Further, time step size increases can be accomplished for the slow moving portions of the transient by utilization of a zero neutron lifetime approximation. Reactivity feedback due to density changes or motion of core constituents is computed by searching input worth tables.

5. Restrictions on the Complexity of the Problem and Uncertainties: Heat transfer calculations for up to 10 radial regions (channels or rings), and 20 axial segments may be performed simultaneously. Radial heat transfer calculations within each pin axial segment are done using up to 12 radial fuel nodes, a gap (or sodium bond) node, and a cladding node and coolant node. Coolant flow within each channel may be specified as a function of time. Point kinetics with up to six delayed neutron precursor groups is used to compute the transient power level.

A point kinetics formulation is used which is probably non-conservative. It is suspected, however, that significantly larger uncertainties are inherent in the present model for molten fuel motion and coolant expulsion. No coolant re-entry model presently exists. Detailed loading on the cladding cannot be done because only one fuel material type is treated and fuel expansion, due to density reduction or fission gas release, is not taken into account. A natural source of pin failure incoherency, due to statistical fluctuations and differing power ratings within subassemblies and ring of subassemblies, is ignored, although the program can be modified to partially account for the latter effect.

6. Related and Auxiliary Programs: MELT-II represents a complete revision of the earlier MELT-I program.⁽¹⁾ The major improvements include a detailed heat transfer package, treatment of variable material properties, and the capability for treating coolant expulsion due to sodium voiding, fission gas release, or a molten fuel-coolant interaction. Further, to facilitate continuity in the analytical investigation of major fast reactor excursions, the MELT-II program has been constructed to directly interface the VENUS two-dimensional core hydrodynamic disassembly program.⁽²⁾ If disassembly conditions are established, the fine structure

temperature information is integrated to conform to the R-Z spatial mesh structure used in VENUS and this input, along with the power distribution and all reactivity feedback components, is used directly as the starting point for the disassembly phase in VENUS. In addition, the core is scanned for liquid sodium content to determine the effective Doppler coefficient and to establish whether a sodium-in or sodium-out equation-of-state should be employed at each particular mesh point in the hydrodynamics calculation.

7. Typical Running Time: Since most of the computation time is associated with the temperature calculation and spatial feedback terms, running time is almost directly proportional to the geometric detail, i.e., the total number of spatial nodes. Several problems have been run using 6 radial channels, 18 axial segments, and a total of 10 radial nodes within the fuel pin. Experience has indicated that computations require approximately one second of UNIVAC 1108 processor time per time step. Hence, a typical loss of flow accident may require approximately 8 minutes and a typical power transient may run in about 4 minutes. These times correspond to cases with a substantial amount of printed output plus plotting. Significant savings can be accomplished by reducing the request for output detail.
8. Unusual Features of the Program: The basic philosophy in constructing the program was to provide a framework for consistently and rapidly testing the importance of various feedback phenomena on the course of an excursion. Hence, the program is quite flexible and can easily be upgraded as better mechanistic models become available. The variable time step feature, guarded by recycle capability if important

effects are originally overshoot, provides for a high degree of efficiency in the program. A wrapup option is included which, upon case completion, will write out all salient data in an ordered chronological fashion. The free format code input package has been found very useful to facilitate restart cases or perform batch runs.

9. Status: Production.
10. Machine Requirements: Computer memory - 64K.
11. Experimental Verification: None.
12. References:
 1. Alan E. Waltar, "MELT-I, A Simplified Meltdown Code for Fast Reactor Safety Analysis", BNWL-944, Battelle-Northwest, Richland, Washington, 1968.
 2. W. T. Sha and T. H. Hughes, "Hydrodynamics Fast Reactor Power Excursion Computer Program", ANL-7701, Argonne National Laboratory, Argonne, Illinois, 1970.

REXCO-H⁽¹⁾

1. Name of Code: REXCO-H. Originator: ANL
2. Computer for which Program is Designed: IBM-360.
Programming Language: Fortran IV.
3. Nature of Physical Problem Solved: The code calculates the two-dimensional hydrodynamic response of primary reactor containment to shock waves emanating from the reactor core after the neutronics have ceased.
4. Method of Solution: The conservation equations of mass, momentum and energy and equations of state of reactor materials have been programmed as finite difference equations. Output is determined for a specified input pressure pulse. For each problem, the code computes the displacements, velocities, pressures, specific internal energies, densities, and strains at every spatial point for a specific time interval. (The output of displacements and pressures also can be given pictorially, showing the movements and deformations or magnitudes of pressures at all spatial points at any instant of time.) These computations are repeated for every time interval until the reactor vessel ruptures or the force acting on the rotating shield plug exceeds the strength of the holddown mechanism, whereupon the computation ceases. Thus, this containment analysis and code give in detail the propagation of shock waves, the loads imposed on different parts of the reactor, and the consequent damage throughout the sequence of the problem.

A special calculational problem exists for flows at the shocks because the dependent variables are no longer continuous as they are without shocks or between shocks.

These shock discontinuities are eliminated, without jeopardizing the conservation laws, by the pseudoviscosity method of von Neumann and Richtmyer.⁽²⁾

5. Restrictions on the Complexity of the Problem: The REXCO-H code only calculates results caused by the first of the two destructive elements in a nuclear excursion. The first element is the initial shock wave: the second is the vapor pressure which is a quasi-static pressure as opposed to the short-duration pressure produced by the shock wave and resulting fluid momentum. Thus, REXCO-H is only valid for times up to about 0.1 sec.
6. Unusual Features: Pictorial displays of the grid displacement and pressure are available by means of an IBM-2280 film recorder. Calcomp displays are also optional.
7. Status: REXCO-H is available as a production code.
8. Experimental Verification: REXCO-H results have been compared to experimental data from the reactor explosion tests performed by UKAEA at Foulness and to other European test results. The results of the comparison show good agreement with each of these experiments.
9. References:
 1. Yao-Wen Chang, Joseph Gvildys, and Stanley H. Fistedis. "Two-Dimensional Hydrodynamics Analysis for Primary Containment", ANL-7498, Argonne National Laboratory, November 1969.
 2. J. von Neumann and R. D. Richtmyer. A Method for the Numerical Calculation of Hydrodynamic Shocks, J. Appl Phys. 21, No. 3, 232-237, March 1950.

RIBD-II

1. Name of Code: RIBD-II. Originator: HEDL
2. Computer for which Program is Designed: UNIVAC 1108.
Programming Language: Fortran IV.
3. Nature of Physical Problem Solved: RIBD⁽¹⁾ calculates isotopic concentrations resulting from two fission sources (e.g., ^{238}U and ^{239}Pu) with normal down-chain decay by beta emission and isomeric transfers and interchain coupling resulting from (n,γ) reactions. The calculations follow the irradiation history through an unlimited number of step changes of unrestricted duration and variability including shutdown periods, restarts at different power levels and/or any other level changes

Output consists of isotopic concentrations, activities, beta powers, gamma powers, and energy releases for the specified decay times.
4. Method of Solution: RIBD-II is a grid processor that will handle a library containing 770 isotopes with provision for direct yields from two fission sources, interchain coupling by neutron capture, and that will follow the irradiation history through an unlimited number of power changes including outages. The buildup portion differs from other codes in that it does not use the Bateman equations for its solution form and is therefore not limited to simple, nonbranching chains. The concentration of each nuclide is calculated from a choice of three alternate series solutions depending on the magnitude of the parameters involved. During shutdown decay calculations, when neutron capture is not possible, equations with characteristics similar to the Bateman equations are used.

5. Restrictions on the Complexity of the Problem and Uncertainties: Isotopic ground states are allowed to have no more than seven source paths. Up to five source paths are allowed for isomeric states. No upchain processes are allowed ($n-\alpha$, $n-p$, $n-2n$, α or β^+ emission). No beta decay is allowed from one isomeric state to another isomeric state.
6. Related and Auxiliary Programs: RIBD-II is an extension of the RIBD⁽¹⁾ code. Calcomp plotting routines are available for plotting RIBD results.
7. Running Time: Case dependent. 4 steps of power, 10 decay times, and 770 isotope inventory requires about 90 second.
8. Unusual Features: RIBD calculates an inventory with two fission sources, accounting for differential burnup, while permitting a flexible operating history to be followed. The decay schemes of the radionuclides are accurately duplicated by the code. Neutron-induced transmutation of fission products are included.
9. Status: RIBD-II is in production at HEDL; RIBD is available through the Radiation Shielding Information Center at ORNL.
10. Machine Requirements: 65K memory.
11. Other Programming or Operating Information or Restrictions: A 770 isotope master library has been developed for use with RIBD-II. The user has the choice of the yields of Zysin, et al,⁽²⁾ Anderson⁽³⁾, or Weaver, et al.⁽⁴⁾ for thermal, fission spectrum, or 14 MeV neutrons. Thermal or FTR core-spectrum weighted cross sections are available.
12. Experimental Verification: Employing Anderson⁽³⁾ yield data, the calculations adequately predict decay heat of ²³⁹Pu in the decay range 40 to 150 days as calorimetrically measured by Johnston.⁽⁵⁾

Good agreement is obtained with the gamma decay powers measured by Fisher and Engle⁽⁶⁾ in the time period 0-45 seconds following fission of ^{239}Pu . Calculations agree with Levochin and Sokolov⁽⁷⁾ activity data for both ^{239}Pu and ^{235}U thermal-neutron induced fission in the time range 2 hours to 1 year.

13. References:

1. R. O. Gumprecht. "Mathematical Basis of Computer Code RIBD", Dun-4136, June 17, 1968.
2. Y. A. Zysin, A. A. Lbov, and L. I. Sel'chenkov. "Fission Product Yields and their Mass Distribution", Consultants Bureau, New York, N. Y., 1964.
3. C. A. Anderson, Jr. "Fission Product Yields from Fast Neutron Fission of ^{239}Pu ", LA-3383, Los Alamos, New Mexico, December 1965.
4. L. E. Weaver, P. O. Strom and P. A. Killeen. "Estimated Total Chain and Independent Yields for Several Neutron Induced Fission Processes", USNRDL-TR-633, March 1963.
5. K. Johnston. "A Calorimetric Determination of Fission Product Heating in Fast Reactor Plutonium Fuel", J. of Nuc. Eng., Vol. 19, pp 527-539, 1965.
6. P. C. Fisher and L. B. Engle. "Delayed Gammas from Fast Neutron Fission of U^{232} , U^{233} , U^{235} , U^{238} , and Pu^{239} ", Phys. Rev., Vol. 134, #4B, May 1964.
7. F. K. Levochin and Y. Y. Sokolov. "Change in the Activity of U^{235} and Pu^{239} Fission Products with Time", Atomnaya Energiya, Vol. 10, pp 403-404, April 1961.

SASIA⁽¹⁾

1. Name of Code: SASIA. Originator: ANL.
2. Computer for which Program is Designed: IBM-360 and CDC-3600.
Programming Language: Fortran IV.
3. Nature of Physical Problem Solved: SASIA⁽¹⁾ is a fast reactor neutronics - heat transfer accident analysis program designed to accurately simulate fuel pin behavior and voiding phenomena within a subassembly during a major accident. Further, phantom channels are included which utilize extrapolation procedures to allow behavior in several radial regions of the core to be estimated. Once core disassembly conditions are established, a core radial power profile is read in and the accident simulation can be continued using a modified version of the MARS⁽²⁾ core disassembly program.

Models are included for nuclear kinetics (point model), Doppler feedback, fuel expansion, coolant density change, structural effects, and coolant voiding (two phase flow and slug flow models).

4. Method of Solution: Heat transfer calculations are accomplished using the implicit Crank-Nickolson scheme. Hence, a variable time step routine can be used to optimize program efficiency. An interaction loop is built around Doppler feedback to insure that the selected time step is compatible with accuracy in the power calculations. Continuity and momentum equations are solved each time step for the two phase coolant boiling routine until a preset void fraction in the coolant is reached. Beyond that time, a slug ejection model can be used. Reactivity feedback is computed using perturbation theory, i.e., input worth tables are searched once appropriate material motions have been established.

5. Restrictions on the Complexity of the Problem and Uncertainties:

Heat transfer calculations within a pin may be performed for up to 20 axial segments, each being comprised of up to 15 fuel nodes plus 3 cladding nodes and a single node for the coolant and structure. In the disassembly phase, up to 60 material regions can be accommodated and the maximum R-Z mesh is 20 x 20. Detailed heat transfer calculations are restricted to a single pin so that whole core behavior can only be estimated using an extrapolation procedure.

A point kinetics formulation is used which is probably non-conservative. It is suspected, however, that significantly larger uncertainties are inherent in the present model for molten fuel motion and coolant expulsion. No coolant re-entry model is included in the present version. Detailed loading on the cladding cannot be done because only one fuel material type is treated and fission gas release effects are not taken into account. Fuel density reduction due to thermal expansion, however, is treated. A natural source of pin failure incoherency, due to statistical fluctuations and differing power ratings within subassemblies is ignored. Reactivity feedback due to coolant expulsion is very difficult to estimate since only conditions within a single fuel pin are explicitly calculated.

6. Related and Auxiliary Programs: SAS1A represents the first completed computer package of the Safety Analysis System coding system. An updated multi-channel version of SAS1A is under active development and is known as SAS2A. The disassembly phase calculations of the SAS1A program are carried out by a modified version of the MARS program⁽²⁾.

7. Typical Running Time: Running time is understood to be of the order of 1/2 seconds of IBM-360 (mod. 75) central processor time per time step for a slow power transient in which the geometric structure includes approximately 12 radial pin nodes and 15 axial segments. This results in a computation time of three to four minutes up to the point of disassembly and about 1/2 minute additional for the disassembly phase.
8. Unusual Features: Prior to cladding rupture, radial fuel expansion and eventual cladding strain is explicitly calculated. When a specified amount of fuel melting has occurred, a special subroutine can be used to compute some axial motion of molten fuel. Cladding loading due to fission gas release is not included in the original version but is being formulated for future versions. A two phase flow model is included to simulate coolant boiling for conditions of low initial superheat.
9. Status: Production. Available through the Argonne Code Center.
10. Machine Requirements: IBM-360 ~ 450K bytes
CDC-3600 ~ 50K words
11. Experimental Verification: A modified version of the SAS1A code, which is designated as SAS1A-ASH, has been prepared exclusively for analysis of fuel-meltdown experiments in the TREAT reactor. Results of this effort have been reported.^(3,4,5)

Although it is too early to arrive at any solid conclusions, to date the correlations of SAS1A-ASH predictions to actual TREAT experiments have been generally satisfactory for unirradiated fuel pins. For example, a PFR pin was predicted to survive a recent TREAT transient with little cladding deformation and, indeed, the pin did survive with even less strain than predicted. A PNL pin was predicted to fail due to coolant boiling and early

post-test examination appears to confirm this. However, numerous phenomena are involved in tests of this type and generalization can be misleading. Suffice it to say that, based on early testing, the program shows considerable promise.

12. References:

1. G. J. Fischer, et al. "Fast Reactor Accident Study Code SAS-1A", Conf. Effective Use of Computers in the Nuclear Industry, Oak Ridge National Laboratory, 1969.
2. N. Hirakawa. MARS, A Two-Dimensional Excursion Code, APDA-198, Atomic Power Development Associates, Inc., June 1967.
3. A. K. Agrawal. Trans. Am. Nucl. Soc., 12, 865, 1969.
4. A. B. Rothman. Trans. Am. Nucl. Soc., 13, 652, 1970.
5. C. E. Dickerman. "Reactor Development Program Progress Report", ANL-7737, Argonne National Laboratory, 1970.

SOCOOL-II⁽¹⁾

1. Name of Code: SOCOOL-II. Originator: HEDL.
2. Computer for which Program is Designed: UNIVAC 1108.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: SOCOOL-II calculates the conversion of thermal to mechanical work energy when a molten material is instantaneously mixed with sodium.
4. Method of Solution: Spherical particles of the molten material are assumed to be instantaneously and uniformly dispersed in the sodium. The mixing region is surrounded by unheated sodium. The rate of heat transfer is obtained by solving the heat conduction equation in spherical coordinates using the implicit numerical method. Assuming that the unheated sodium is compressible, the expansion of the heated sodium is calculated using the one-dimensional acoustic equation.⁽²⁾ Boiling conditions are attained when sufficient expansion relieves the high pressures generated by rapid heating. Boiling is assumed to vapor-blanket the hot material and prevent further heat transfer and the heated sodium is then isentropically expanded to a specified pressure. The acoustic work is calculated by integrating under the pressure-volume curve until boiling conditions are attained. The inertial work is obtained from the thermodynamic isentropic expansion process.
5. Restrictions on the Complexity of the Problem and Uncertainties: The code does not consider the effect of initial gas or vapor voids on compressibility and heat transfer. It does not allow for finite rate of fragmentation and dispersal of the molten material into the sodium.

6. Related and Auxiliary Programs: At the present time, the code contains a dummy subroutine for plotting the results.
7. Running Time: Typical running time is 10 seconds.
8. Unusual Features: The properties of the molten material can be specified as input but the properties of approximately 25% PuO_2 to 75% UO_2 are self-contained in the code. The thermal and mechanical properties of sodium can be specified as input if they are to be assumed constant but three different schemes for calculating variable sodium properties are self-contained in the code.^(3,4,5)
9. Status: The code is operational at the AEC Richland Operations Computer Facility operated by Computer Sciences Corporation.
10. Machine Requirements: Memory requirements not large.
11. Other Programming or Operating Information or Restrictions: Fortran V is in use only for UNIVAC 1108 computers operated by Computer Sciences Corporation.
12. Experimental Verification: Experimental data to date indicates that the work energies calculated using SOC00L-II are conservative by an order of magnitude or more. However, the code is not presently set up to utilize the experimental data to calibrate the analytical results.
13. References:
 1. A. Padilla, Jr. "Transient Analysis of Fuel-Sodium Interaction", ANS Transactions, Vol. 13, No. 1, June 1970.
 2. R. H. Cole. Underwater Explosions, Dover Publications, New York, 1948, p 19.

3. G. H. Golden and J. V. Tokar. Thermophysical Properties of Sodium, ANL-7323, Argonne National Laboratory, August 1967.
4. D. Miller, et al. "Estimation of Vapor and Liquid Density and Heat of Vaporization of Alkali Metals to the Critical Point", Paper presented at the International Conference on the Safety of Fast Breeder Reactors, Aix-en-Provence, France, September 19-22, 1967.
5. Reactor Development Program Progress Report, August 1969, ANL-7606, Argonne National Laboratory, p 131.

SOFIRE-II

1. Name of Code: SOFIRE-II. Originator: AI.
2. Computer for which the Program is Designed: UNIVAC 1108.
Programming Language: Fortran V.
3. Nature of Physical Problem Solved: SOFIRE-II calculates sodium pool burning dynamics and the accompanying thermal transients in gas atmosphere and in the enclosing structure and over-pressure in the cell.
4. Method of Solution: March-out type calculation computes time and temperature dependent mass transfer⁽¹⁾ of oxygen to the sodium surface, natural convection heat transfer⁽²⁾ from gas to structure, radiation heat transfer from pool to walls and an additional empirically determined quasi-radiation term⁽³⁾ from pool to gas. For the pool and structures the one-dimensional Fourier transient conduction equation is solved. In addition to the sodium pool and heat storing masses in each cell there are three heat structures representing the primary cell and two heat structures for the secondary cell. Any of these components may be omitted if desired. Each heat structure has nine temperature nodes in series. Thermodynamic relations on the gas space assume an ideal gas.

An optional two-cell case may be calculated with the second cell located above the primary cell where burning takes place. The duct opening between cells has a specified cross-section, diameter and length. The flow between cells is computed by balancing the static pressure difference (higher in the cooler upper cell) against the buoyancy due to the temperature difference (higher in the lower cell).

The calculation is termed a "one-cell" case if the second cell is not included.

Output is in paragraphs of data for selected printout time-steps. Gas temperature and pressure, oxidation conditions and structure temperatures are listed.

5. Restrictions on the Complexity of the Problem and Uncertainties: The solution becomes unstable for very small sodium spills, i.e., the pool depth should be $>1/2$ -in., or zero (no sodium). Programmed for liquid sodium the code does not allow for calculation in the phase transition, solid or vapor phase. Thermal characteristics of materials are assumed constant throughout the calculation. Errors so introduced are usually not detrimental since temperature variations are moderate. The input capacities for heat structure elements and the input values of admittance between them are the major quantities affecting results and these are, of course, controlled by the user. Tests on the "two-cell" option indicate that the stepwise inflow to the primary cell relative to the volume of the cell is the approximate error to be expected in calculated pressure and temperature of the gas and heat structures, i.e., a ratio of 5% inflow results in ~5% overestimate of pressure and temperature.
6. Related and Auxiliary Programs: For the purpose of determining radiological and siting requirements for sodium cooled reactors the SOFIRE-II code calculates release of airborne oxides versus time. This is the input quantity for calculation of aerosol fallout transients using the HAA-3A code.

7. Running Time: The typical "one-cell" case runs at 1 second/hr of real time. The running time for the "two-cell" case is implicitly configuration dependent. Explicitly, the stepwise inflow to the primary cell (burning region) should be limited to ~5% of the volume of the primary cell (see Para. 5). A typical case for a 30,000 ft³ primary cell with 100 ft² opening to a 1 million ft³ secondary cell runs at 8 seconds/hr of real time.
8. Unusual Features: Heat release by self-absorption in the sodium pool due to γ -active ²⁴Na is included by option. Selective releases of fission product decay heat may be accounted for in gas, sodium and structure. Values of input parameters will simulate normal operation or a prior accident, such as sodium spray fire. In such a case there may not actually be a sodium pool fire, only a heat transfer problem accommodated with no sodium pool present. A useful option is the NAMELIST (UNIVAC 1108) input for running parametric cases as alternates on the base data set.
9. Status: The program is now in operation at HEDL.
10. Machine Requirements: Approximately 35K of memory required.
11. Other Programming or Operating Information or Restrictions: Originally written for the IBM-360 by Atomics International,⁽⁴⁾ the present UNIVAC 1108 Fortran V version may be easily converted to other Fortran operating systems.
12. Experimental Verification: A continuing program of experimental verification is progressing at Atomics International.⁽³⁾ It was due to this program that a basic change in the original pool fire calculation, SOFIRE-I, was made⁽⁴⁾ and resulted in

the more realistic and more concise calculation now called SOFIRE-II. All of the resultant parameters for pool burning in the "one-cell" case have been verified to within a few percent.

13. References:

1. R. B. Bird, W. E. Stewart and E. N. Lightfoot. Transport Phenomena, John Wiley & Sons, 1960.
2. E. R. G. Eckert and R. M. Drake, Heat and Mass Transfer, McGraw-Hill Book Co., New York, 1959.
3. H. A. Morewitz, et al. Annual Technical Progress Report, LMFBR Safety Programs, GFY 1969, AI-AEC-12858 (Health and Safety), Atomics International, Canoga Park, California, October 15, 1969.
4. R. P. Johnson, et al. "Characterization of Sodium Pool Fires", Proc. Conference on Sodium Technology Large Fast Reactor Design, November 7-9, 1968, Part I, ANL-7520, Argonne National Laboratory, Argonne, Illinois, 1968.

VENUS^{*}

1. Name of Code: VENUS. Originator: ANL.
2. Computer for which program is Designed: UNIVAC 1108.^{*}
Programming Language: Fortran IV.
3. Nature of Physical Problem Solved: VENUS is a two-dimensional coupled neutronics-hydrodynamics program to simulate the disassembly phase of a major fast reactor excursion.⁽¹⁾
Equations of continuity and momentum are solved for a reactor modeled in R-Z geometry, wherein the material is assumed to behave as a nonviscous fluid. Since a density dependent equation-of-state can be accommodated, the program is able to simulate a wide variety of accident conditions.
4. Method of Solution: The reactor is modeled in R-Z geometry using a Lagrangians coordinate system, i.e., the grid structure floats with the moving mass. The momentum equations are solved using a Taylors series approximation for the pressure gradients, in which the pressures used in the evaluation are determined at the midpoint between spatial meshes. A pseudo viscosity term, developed by von Neumann and Richtmyer,⁽²⁾ is included to effectively smear out the shock front and improve numerical stability. Point kinetics used to describe the neutronic behavior and a spatial weighting scheme is used to compute Doppler feedback. The equation-of-state package is quite flexible; local pressures can be computed as a function of local fuel temperatures and fuel density.

^{*}This program was originally developed at ANL for the CDC-3600 and the IBM-360 (Mod. 75).⁽¹⁾ The description here contained represents only the version as modified and operable on the UNIVAC 1108.

5. Restrictions on the Complexity of the Problem and Uncertainties:
The present program version can accommodate a reactor description including a maximum of 18 different material regions, each with maximum radial and axial mesh structures of 26×26 , and a total outer R-Z mesh structure of 50×50 . However, the product of outer R-Z nodes cannot exceed 841. Since the hydrodynamic equations are formulated for a nonviscous fluid, the program is only relevant, in its present form, to core situations where sufficient melting has occurred that structural effects are not important. As with any program utilizing a Lagrangian coordinate system, VENUS does not render meaningful results if too much mesh distortion takes place.

A point kinetics formulation is used which is probably non-conservative. It is suspected, however, that significantly larger uncertainties are inherent in the treatment of moving mesh points and the equation-of-state. Structural effects are completely ignored; the material is assumed to behave as a non-viscous fluid. The effect of the reflector on total energy generation, pressure distribution, etc., has not been thoroughly examined. The equation-of-state although quite flexible in allowing for pressure fluctuations as a function of fuel density as well as fuel temperature, is not well defined. Any heat transfer effects during the disassembly phase are ignored.

6. Related and Auxiliary Programs: Since VENUS is formulated for a nonviscous fluid material system, it is important to be able to specify reasonable core conditions, e.g., temperature distributions and melting patterns, at the time hydrodynamic effects physically become important. Hence, VENUS has been modified to accept input directly from the MELT-II program at the time core disassembly conditions are established. For this starting point,

neutronics balance is accomplished and core temperature and power distributions are transferred. Further, the core is scanned for liquid sodium content to determine the effective Doppler coefficient and to establish whether a sodium-in or sodium-out equation-of-state should be employed at each particular mesh point in the hydrodynamics calculation. Plans are being made to link VENUS with other pre-disassembly programs such as SAS-2A and FREADM-1.

7. Running Time: Several cases have been run using nine material regions and a R-Z structure comprising 16 x 28 nodes. For this situation, a complete neutronics-hydrodynamics time cycle appears to consume approximately 1.3 seconds of UNIVAC 1108 central processor time. Since most excursions can be simulated by about 100 steps, this corresponds to about two minutes of computation time. More time steps are usually required if it is desired to monitor the pressure distribution in detail.
8. Unusual Features: Two-dimensional simulation of the reactor in Lagrangian coordinates allows analysis of reactor behavior for sodium-in conditions and for situations wherein asymmetric effects can be important. For example, potential fuel implosion associated with the discontinuous power distributions in a zoned core is automatically treated. Likewise, inclusion of an equation-of-state appropriate to a core with locally voided regions can easily be accommodated. The ability of the program to start from a non-equilibrium partially molten core condition allows interfacing with a pre-disassembly transient program and, thereby, allows the analyst to reduce much of the arbitrariness normally associated with core disruptive calculations. Since the same

rapid variable time step neutronics package that exists in the MELT-II program is contained in the HEDL version of VENUS, time steps can be maximized for very efficient computer usage.

9. Status: Production.
10. Machine Requirements: Computer memory - 64K.
11. Experimental Verification: None.
12. References:
 1. W. T. Sha and T. H. Hughes. "VENUS - A Two-Dimensional Coupled Neutronics-Hydrodynamics Fast Reactor Power Excursion Computer Program", ANL-7701, Argonne National Laboratory, Argonne, Illinois, 1970.
 2. J. von Neumann and R. D. Richtmyer, J. Appl. Phys., 21, 232, 1950.

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