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WANL NUCLEAR EXCURSION ANALYSIS PROGRAM (Title Unclassified)

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April 29, 1964

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Subject: WANL-TME-735, WANL Nuclear Excursion Analysis Program, April 1, 1964

Dear Mr. Schroeder:

Transmitted herewith are three (3) copies of the subject report.

This report is transmitted for your information.

Respectfully,

2. F. Faught

H. F. Faught Program Manager NERVA Nuclear Subsystem

Enclosures - 3

cc: Mr. R. Wilke, SNPO-C Resident Office at WANL







WANL NUCLEAR EXCURSION ANALYSIS PROGRAM (Title Unclossified)

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INTRODUCTION

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The recognition of the potential accidents associated with a nuclear rocket engine is of utmost importance to the safety requirements of the NERVA program. The more severe of these accidents will involve an abrupt increase in core reactivity and an ensuing nuclear excursion. Appropriate safeguards in design and procedure will be used to lessen or eliminate the possibilities of such accidents. Although such safeguards can be extremely reliable, some chain of events can in some cases be postulated which could render them ineffective or inadequate. It is, therefore, necessary to assume highly improbable conditions to predict the intensity of accidents so as to adopt extra precautionary measures for safety.

The ultimate objective of the WANL excursion analysis program is to develop a generalized analytical model which predicts the biological hazards resulting from any conceivable accident involving a nuclear excursion occurring at any phase of the NERVA program. These hazards will arise primarily from the exposure of an involved population to radioactive fission products. The exposure can be effected either through ingestion and inhalation of radioactive core particles or downwind "cloud" doses as a result of fission product gases which have diffused from the core.







ANALYTICAL APPROACH

The following parameters must be incorporated in a meaningful generalized analytical model.

- 1. The core characteristics and existing fission product inventory prior to an excursion.
- 2. The mode and rate of reactivity insertion, e.g., control drum failure, core compaction upon impact with the ground, hydrogen propellant flooding due to a turbopump failure on the launch pad, immersion and flooding with water.
- The shutdown mechanisms involved in terminating the excursion, e.g., temperature (Doppler effect and change of thermal base), density (effect on neutron mean free paths), vaporization and core break-up (increased leakage).
- 4. The core temperature distribution with time both during and after the excursion and the gradients encountered across the pyrolytic coating of the fuel beads.
- 5. The fission product release through diffusion both during and after the excursion.
- 6. The downwind cloud doses due to the diffused fission product gases.
- 7. The physical characteristics of the core after shutdown. Upon break-up, the size, distribution and activity of the particles.

Thus, a generalized analytical model must incorporate nucleonics, hydrodynamics, thermodynamics with transient heat flow, dynamics, and the fission product inventory with diffusion. WANL has developed and is developing several computer programs appropriate to the problem areas defined above. Eventually, they will be combined and integrated into a generalized excursion analysis program applicable to any conceivable accident. A description of these programs is given below.









Figure 1 Block Diagram of Experimental and Analytical Integrated Reactor Excursion Analysis Program







EXPERIMENTAL PROGRAM

Many of the parameters involved in the anticipated excursion analysis program defy a purely analytical approach and must rely to some extent on empirical data. A list of experiments (completed, partially completed, and anticipated) required to complement and test the validity of the analytical model includes:

- 1. Electrical transient
- 2. Water immersion
- 3. Core compaction
- 4. SWET tests
- 5. SPERT tests
- 6. TREAT tests

A block diagram showing the relationship between the experimental and analytical work is shown in figure 1.

Experimental work on electrical transients ¹ and core compaction ² has been temporarily interrupted. Testing in these areas will continue as soon as possible so that these data will be available as input to the excursion analysis program.





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Figure 2 Neutronics - Hydrodynamics Combined







COMPUTER PROGRAMS

A description of the two existing programs: VARI-QUIR and NECKLACE and the two under development, NERVEX and FIPDIF is given below. They are being incorporated into WANL's Integrated Excursion Analysis Program. A more detailed description of these programs is given in the references.

a. <u>VARI-QUIR</u> VARI-QUIR^{3,4} is written in FORTRAN for the IBM-7094 computer. The program solves the non-separable neutron kinetics problem using diffusion theory in two dimensions with up to four neutron energy groups and six precursor groups. It is based on a variational calculus approach in conjunction with an assumed guadratic spatial dependence per region with time varying coefficients.

Such a non-separable solution (i.e., the spatial dependence of the neutron flux can depend on time) is particularly desirable for predicting the core behavior and fission product release during a nuclear excursion resulting from water immersion. The increased moderation due to the introduction of water causes a marked change in the neutron spatial dependence and consequently the relative fission energy generation throughout the core.

The neutron kinetic behavior is dictated by either specifying input reactivity or cross section variation with time via a series of ramps. Thus, control drum failure is described using the known reactivity worth of the drum positions and specifying a rotation rate. On the other hand water immersion is described by altering the cross-section in the appropriate core region dictated by the rate of water insertion.

VARI-QUIR is now being expanded so as to include negative reactivity feedback effects contributing to shutdown. This feedback will operate through the cross-section variations associated with changes in density and temperature (thermal base and Doppler effect) changes. These will be obtained from the hydrodynamics (see NERVEX description) portion of the anticipated excursion program. A block diagram showing how the neutronics and hydrodynamics will be combined is shown below in figure 2.

b. NECKLACE

NECKLACE⁵ is another of the series of computer programs coded for the RAC (Reactor Accident Calculation) series, (Beads Around Neck). It was originally named RAC-H. After the publication of RAC⁶ it became NKLS, NEK-2, and lastly, NEK-4.







NEK-2 is coded in FORTRAN-II for the Los Alamos 7094 computer. NEK-4 is identical to NEK-2 except that it is coded in FORTRAN-IV for the Los Alamos IBM 7030 STRETCH computer. It is expected that NEK-4 will be compatible with FORTRAN-IV assembly procedures on the 7094.

Like all the programs of the RAC series, NEK is a "first-step" effort, designed only to aid "educated guessers" to evaluate the possible consequences of uncontrolled transients in small, high-power systems. It is an attempt to look at the transient behavior of the microscopic fuel beads which may make up the active material of newer fuel elements.

The mathematics methods in NEK are crude and simple but justifiable by the lack of information in all properties of materials at the expected temperatures and transient conditions.

The NECKLACE code attempts to describe the transient heat, hence temperature, distribution in a system of spherical fuel materials imbedded in graphite. Fissions are assumed to take place in a central region in which most of the heat is generated by stopping the fission products. Some products escape across the boundary into non-fissionable materials so allowance is made for some heat generation there.

This code will be utilized in WANL's excursion analysis program for those cases where it is applicable, i.e., reactivity insertion rates and power depositions great enough to fragment the fuel.

c. NERVEX

At present, the hydrodynamics portion of the WANL excursion program utilizes the one dimensional computer program (RAC)⁶ developed at Los Alamos. RAC assumes a homogeneous continuous core whose behavior is described by a time dependent fluid flow model but with the ability to sustain both compression and tension. Core expansion is restricted to the axial direction and shutdown is realized through temperature and density changes. WANL is now formulating a more general twodimensional hydrodynamic model which will include radial expansion contributing to shutdown. This formulation will be programmed in FORTRAN for the IBM 7094 computer and will then be coupled with the VARI-QUIR program. Much of the formulation has been completed and is described below. The completed program is referred to as the NERVEX program.

The NERVEX formulation is based on a time dependent quasi-fluid flow model wherein the core is assumed to be homogeneous perfectly elastic, but anisotropic. The anisotropy follows since the fuel elements are aligned axially. This alignment will prevent tensions from being sustained radially and shears axially. This model considers the simultaneous solution of the momentum equations in







radial and axial directions, the energy equation, equation of state, and continuity of mass equation. The Von Neumann-Richtmyer pseudo-viscous shock pressure is also included in the event shock waves arise during the excursion duration. If the reactor core should impact upon ground or water, it is not unlikely that shock waves might arise. Due to the intended purpose of the NERVEX program, in which computer storage may be restrictive, an explicit rather than an implicit (requiring iterations) finite difference approach will be used to solve the fluid flow equations. Such an approach is usually based on either the Eulerian or Lagrangian forms of the equations. In the Eulerian approach, the independent space variables refer to a fixed coordinate system and the fluid motion is described by a time dependent velocity field. In the Lagrangian approach, the independent space variables refer to a coordinate system moving with the fluid and the fluid motion is described by the time behavior of these space variables. The Lagrangian approach has been used for this formulation due to the following advantages over Eulerian.

1. Each mass point can be identified by its original position. This makes possible the treatment of regions with different thermodynamic properties and a direct treatment of boundary conditions such as imposed by the tie rod springs.

2. The conservation of mass is automatic and exact. This is important due to the extreme sensitivity of pressure with density changes.

One of the basic sections of this code to be utilized for prediction of fission product release is that part which predicts the motion and state, i.e., pressure, temperature and density of the reactor material throughout the core.

Since the end goal of this section is to determine realistic parameter values to be used in fission power release calculations special attention must be devoted to considerations of density and temperature. Of primary importance in correct calculation of these values is the two dimensional (r, z) aspect of the core since radial displacements imply twice the density variation as a similar displacement in one dimension. Also, if restrictions are placed upon radial core expansion or contraction then the property values such as the modulus of elasticity and coefficient of thermal expansion available from the usual experiments are not directly applicable to the problem. The "a priori" assumption that pressure gradients and hence momentum considerations are of primary importance in only one particular direction, say, either the radial or the axial direction cannot be made without first ascertaining this fact from a two dimensional (r, z) calculation. Without this calculation it









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appears that the association of properties or displacements in one direction corresponding to properties or displacements in some arbitrary preferential direction must be disallowed.

The above considerations, coupled with the fact that radial variations in reactivity insertion or core characteristics may be of importance led to the present consideration of the two dimensional radially symmetric code model.

The formulation of the NERVEX equations assumes a hydrostatic pressure. At low pressures and slow excursions the thermal expansion, roughly under equilibrium, should dictate the order of events. However, momentum becomes important at the high pressure, fast excursions and under these high pressures the motion of the core corresponds approximately to that of a fluid and hence the stresses are approximately hydrostatic.

Also under consideration are the various failure modes for the fuel rods and the effect of failure upon subsequent motion, the spring loading of the core surfaces, and the vapor and liquid phase generation. These should be completed shortly. Figure 3 shows a simplified flow diagram of NERVEX and illustrates the pertinent calculations involved.

d. FIPDIF

FIPDIF⁷ is a fission product diffusion program which will calculate the inventory of approximately 250 isotopes in a NERVA core and the diffusion of these isotopes from the core under any combination of the following conditions:

- 1. Normal operation
- 2. Normal cooldown
- 3. Accidental loss of coolant
- 4. Nuclear excursion

The core will be divided into a number of equal length sections and diffusion parameters will be calculated for each of four categories of isotopes, which correspond to the fuel temperature in the









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core section. Data accumulated thus far indicates that it may be necessary to divide each of the categories, which will be established according to the relative rates of diffusion of the isotopes, into two or more subcategories for convenience in programming.

In the case of normal operation a previously computed temperature distribution will be input to the program. It will be assumed that the fission power and that which is generated by fission product decay are balanced by the rate of removal of heat by the coolant.

A normal cooldown will be approximated by a series of time increments in which the temperature of the sections are constant and the same assumptions are applied as those used during the normal operation phase. New diffusion parameters will be calculated for each time step corresponding to the temperature distribution at that time.

In case of accidental loss of coolant, the temperature in the segments will be determined by calculating rates of both decay heat production and heat dissipation to the atmosphere. The rate of decay heat production will be calculated directly from the fission product inventories and energies of decay and will thus be reduced as fission product diffusion is enhanced with temperature increase.

The effects of a nuclear excursion will be approximated by step changes in the integrated power and fission product inventories. The resulting temperature increases and vapor generation will be determined and additional fission product diffusion will be calculated as in the case of loss of coolant. Figure 4 is a simplified block diagram showing the inter-relationship of the various parameters calculated in FIPDIF.

The diagram shown in figure 5 can be easily understood with the following brief explanation. Each of the large blocks represents subroutines of the main program. In each subroutine the method of calculating fission product inventory and diffusion will be different (as explained above). The diamonds indicate points of decision as to which subroutine will be called at that point. The result of this decision will be determined by the type of problem to be simulated. The five available choices are listed below.

- If the indicator (IND) is set equal to 1 at the start of the problem, it will indicate a period of normal operation followed by a normal cooldown.
- If IND=2, an excursion and subsequent cooldown (with no coolant flow) will be simulated.









- If IND=3, the diffusion resulting from a period of normal operation, followed by a nuclear excursion, will be calculated.
- If IND=4, a loss of coolant accident, which follows a period of normal operation will be calculated.
- 5. If IND=5, the following sequence will be simulated:
 - a. A period of normal operation
 - b. An excursion (which does not disrupt coolant flow)
 - c. A cooldown (with coolant flow) from the elevated temperatures produced by the excursion.

PRESENT AND FUTURE ACTIVITY

The present approach in formulating the WANL Integrated Excursion Analysis Program is to develop a two dimensional thermodynamic and hydrodynamic model (NERVEX), which consists of the fundamental mechanical equations of momentum, continuity, and energy and state. In addition, provisions are being made in this code for conditions such as material failure, change of phase and shock waves. Concurrent with this activity is the integration of the RAC⁵ code, which is a one dimensional description of the thermodynamic and hydrodynamic behavior of a uranium-graphite core during a nuclear excursion, and the VARI-QUIR code which describes the neutron kinetic behavior of a reactor under similar conditions. When the integration and debugging of these two codes is completed in about mid-April 1964 at least two items of interest will be run: water immersion and core compaction.

Shortly thereafter, the two dimensional NERVEX code should be debugged and ready for integration with the two dimension VARI-QUIR code. The experience gained in combining the RAC and VARI-QUIR codes will be, of course, invaluable in expediting the integration of the two dimensional codes. Sample problems will again be run and compared with the answers obtained from the one dimensional model code. The answers obtained from the two dimensional model will be more accurate since it is a better representation of the physical reactor and less conservative than the one dimensional model. A series of mathematical models describing the neutron kinetics, hydrodynamics, heat transfer characteristics, and equations of state of the reactor materials during and after an excursion are required before a meaningful integrated excursion analysis program can be written.









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The various parameters for which mathematical models must be developed and their relationship to each other is shown in figure 6. Also given are the existing codes which with modifications will describe these parameters for the types of excursions of interest. This phase of the development of the WANL²Integrated Excursion Analysis Program should be completed about the end of September 1964.

It is recognized by all that much improvement could be made in such an approach as RAC, other than just the need for a two dimensional treatment. The more obvious of these are as follows:

- a. Vapor is assumed to be confined to the immediate region where generated. Such an assumption should be examined in detail since if vapor were to escape through the coolant channels and perhaps redeposit on cooler surfaces, shutdown would be delayed with a consequent larger fission energy release.
- b. No vapor is assumed to be absorbed in the graphite matrix whereas such an absorption would again delay shutdown.
- c. It is assumed that the fuel beads and the graphite matrix are in thermal equilibrium. For accidents involving short periods there will probably be a significant temperature gradient across the pyrocoating of the beads which will enhance early vapor formation and hence early shutdown. This problem will be handled by the incorporation of the NECKLACE code into the integrated code.
- d. The graphite vapor is assumed to obey perfect gas laws.
- e. Vaporization rate is dictated by an assumed equilibrium with the graphite phase diagram whereas non-equilibrium states may be realized.

An intensified effort for improvement in these areas is anticipated after the two dimensional model is completed.

The next and last phase in the development of the WANL Integrated Excursion Analysis Program will be the incorporation of the FIPDIF program which will define the biological hazards as a result of an excursion.





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