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Thermal-Spectrum Recriticality Energetics

Prepared for the U.S. Department of Energy
Office of Environmental Restoration and
Waste Management

Westinghouse
Hanford Company Richland, Washington

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THERMAL-SPECTRUM RECRITICALITY ENERGETICS

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ABSTRACT

Large computer codes have been created in the past to predict the energy release in hypothetical core disruptive accidents (CDA), postulated to occur in liquid metal reactors (LMR). These codes, such as SIMMER, are highly specific to LMR designs. More recent attention has focused on thermal-spectrum criticality accidents, such as for fuel storage basins and waste tanks containing fissile material. This paper presents results from recent one-dimensional kinetics simulations, performed for a recriticality accident in a thermal spectrum. Reactivity insertion rates generally are smaller than in LMR CDAs, and the energetics generally are more benign. Parametric variation of input was performed, including reactivity insertion and initial temperature.

INTRODUCTION

Best-estimate accident simulation is a mature field as related to liquid metal reactors (LMR). Large computer codes have been written, such as the VENUS and S_N , Implicit, Multifield, Multicomponent, Eulerian Recriticality¹ (SIMMER) codes. These codes simulate the coupled multigroup neutronics, with liquid sodium fluid dynamic feedback. SIMMER in particular treats multiple thermal hydraulic channels, and tracks material component redistribution as the simulated transient progresses. However, there are numerous accident scenarios that can be postulated that occur in thermal neutron systems. These include well-moderated ex-reactor criticality accidents, accumulation of fissile material into a critical configuration inside a waste tank, and water reflood of a damaged light water reactor (LWR) core (such as Three-Mile Island) with water that is insufficiently borated.

Previous recriticality energetics analyses dealing with the conversion of the WNP-1 reactor to a tritium production facility, revealed a lack of sophisticated simulation tools for LWRs, or thermal-spectrum systems in general. It was found that although detailed core melt simulations had been performed in connection with loss of coolant accident (LOCA) events for LWRs, these scenarios were based on decay heat acting as the thermal source, rather than on fission power (i.e., there was no coupled simulation code available that modeled transient neutronics with fluid

dynamics and material redistribution in the way SIMMER does for a fast-spectrum system.) Other hypothetical criticality events investigated at the Hanford Site have included criticality in a waste tank. These tanks are large enough, and contain sufficient fissile material (albeit at a highly subcritical average concentration), that a criticality could occur, given some kind of concentrating mechanism (e.g., preferential precipitation). It is thought that in such an event, the reactivity insertion rate at critical would be low enough so that the resulting neutronic transient would be influenced strongly by the evolving thermal currents, thus shutting down the event by fissile material dispersal; fluid flow feedback would likely disperse the critical configuration before enough time elapsed to attain prompt critical.

This paper presents results for a typical space-time accident simulation. This simulation models an accumulation of fissile material debris into a cylinder of fixed radius. This scenario would be the expected result of a reactor LOCA event, with molten fuel relocating at the bottom of the core inside a cylindrical support structure, such as the type employed in heavy-water production reactors. The one space dimension modeled was the radial dimension of the cylinder, which will be referred to from now on as the 'fuel core', or 'core'. The surrounding material is modeled as heavy water. The cylinder height dimensions are modeled as perpendicular buckling leakage corrections to the group-dependent absorption cross sections in the core and heavy-water-reflector regions. Once the steady state is found (by adjusting the core height), the neutronic transient is driven by a time-dependent axial buckling function. As the neutronic transient evolves, a transient, radial-heat-transfer calculation (driven by the radial-heat-source density supplied by local fission power) concurrently updates the temperature in each radial mesh interval. The macroscopic cross-section library accessed by the neutronics is tabulated as a function of temperature, and is interpolated each time step to update local cross sections (on a mesh-by-mesh basis); both thermal and neutronic profiles are mutually coupled. Although Doppler feedback (built into the cross sections) mitigates the transient and causes power peaks, power will continue to rise because more and more molten material continues to accumulate on top (i.e., reactivity insertion continues). The ultimate shutdown mechanism is the melt-through of the cylinder support structure, with subsequent gravity collapse of the fuel column.

DETAILS OF ANALYSIS

The computer code written to perform this simulation, ATHENA, is a one-dimensional, space-time neutron diffusion kinetics code that treats two neutron energy groups, fast and thermal. The spatial dimension is cylindrical; and reactivity is inserted by specifying the fuel debris mass accumulation rate, which causes a linear increase in core height with time. The transient, two-group neutron diffusion equations in cylindrical geometry are

$$\begin{aligned} \frac{1}{v_1} \frac{\partial \phi_1}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r D_1 \frac{\partial \phi_1}{\partial r} \right) + (\Sigma_{a1} + D_1 B_2^2(t)) \phi_1 &= (1-\beta) (v \Sigma_{f1} \phi_1 + v \Sigma_{f2} \phi_2) + \sum_{i=1}^{10} \lambda_i C_i \\ \frac{1}{v_2} \frac{\partial \phi_2}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r D_2 \frac{\partial \phi_2}{\partial r} \right) + (\Sigma_{a2} + D_2 B_2^2(t)) \phi_2 &= \Sigma_{1-2} \phi_1. \end{aligned} \quad (1)$$

Definitions of these terms may be found in the "List of Symbols" following the "References" section. The delayed neutron equations were extended to ten groups for heavy water, to treat photoneutron effects. The delayed neutron equations are

$$\frac{dC_\ell}{dt} = \beta_\ell (\nu \Sigma_{f_1} \phi_1 + \nu \Sigma_{f_2} \phi_2) - \lambda_\ell C_\ell, \ell = 1, \dots, 10. \quad (2)$$

The core height function is calculated as follows:

$$H(t) = H(\tau_0) + \int_{\tau_0}^t \frac{\dot{m}}{\rho_f \pi R^2} d\tau. \quad (3)$$

This core height then is incorporated into a buckling function:

$$B_z^2(t) = \left(\frac{\pi}{H(t) + 2\delta} \right)^2. \quad (4)$$

This function then is added, by group, to the removal cross section of each neutron equation. The macroscopic nuclear cross sections were obtained from the British WIMS-D lattice transport computer code², using the British 69-group fine group library. Cross sections were generated for a lattice cell composed of the fuel debris core, surrounded by a heavy-water moderator, for a series of temperatures up to the boiling temperature of the alloy fuel. To allow ATHENA to treat boiling, the cross sections were extended at the boiling temperature, but for reduced densities. This allowed ATHENA to interpolate cross sections as a function of reduced mixture density during boiling, if the transient progressed to that point.

A single cylinder of the type modeled would not go critical by itself; a nearly coherent melt, with hundreds of these cylinders filling with fuel debris, was predicted to go critical by MCNP³ Monte Carlo calculations. The ATHENA prediction for the critical height was forced to match the MCNP prediction for the finite array of cylinders by adjusting the outer boundary albedo. The albedo value that produced the MCNP critical height was equal to 0.993.

Radial heat transfer within the fuel debris was driven at each radial mesh by the local fission power, determined by the two-group kinetics solution from the previous time step. The heat transfer boundary condition was convective pool boiling at the interface between the cylinder structure and the surrounding heavy-water moderator. The radial heat transfer model was

$$\rho C_p \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} (rk \frac{\partial T}{\partial r}) = q(r, t). \quad (5)$$

NUMERICAL METHODS

Both neutron diffusion and heat transport equations were integrated in time by using finite difference approximations. The neutron diffusion equations were integrated over each mesh point to arrive at a set of coupled algebraic equations. These equations are three-point coupled in space, with another constant coupling to the 'other' group. After performing the requisite algebra, all terms containing the flux at the 'future' time are brought over to the left-hand side, while all terms containing 'present' information (i.e., time step t_j) are collected into the right-hand side, or

$rhs_{g,i,j}$. All results presented in the following section were produced using Crank-Nicolson, or semi-implicit differencing. The form of the system is

$$\begin{aligned} \ell_i \phi_{1,i-1,j+1} + d_i \phi_{1,i,j+1} + u_i \phi_{1,i+1,j+1} + do_i \phi_{2,i,j+1} &= rhs_{1,i,j} \\ \ell'_i \phi_{2,i-1,j+1} + d'_i \phi_{2,i,j+1} + u'_i \phi_{2,i+1,j+1} + do'_i \phi_{1,i,j+1} &= rhs_{2,i,j} \end{aligned} \quad (6)$$

By staggering the fast and thermal fluxes, it is possible to write this system in the form of a five-diagonal matrix, as follows:

$$\begin{bmatrix} \dots & \ell_i & 0 & d_i & do_i & u_i & 0 & \dots \\ \dots & 0 & \ell'_i & d'_i & do'_i & 0 & u'_i & \dots \end{bmatrix} \begin{bmatrix} \phi_{1,i-1} \\ \phi_{2,i-1} \\ \phi_{1,i} \\ \phi_{2,i} \\ \phi_{1,i+1} \\ \phi_{2,i+1} \end{bmatrix}_{j+1} = \begin{bmatrix} \cdot \\ \cdot \\ rhs_{1,i} \\ rhs_{2,i} \\ \cdot \\ \cdot \end{bmatrix}_j \quad (7)$$

Because of the stiff nature of the kinetics equations, this approach allows for a simultaneous solution of both fast and thermal equations for time step t_{j+1} . The neutronic time step therefore is performed using a single forward-elimination, backward-substitution method, optimized for a five-diagonal matrix (i.e., advantage is taken of all zeros off the five non-zero diagonals).

The radial heat transport equation was solved in a similar fashion. However, a 'staggered mesh' was used. The neutron equations were solved for the mesh points, using finite difference equations that were generalized for different macroscopic cross sections on either side of the mesh point, but the temperature field was calculated for the mesh interval between mesh points. As the average temperature of the cell increased, this information was used to interpolate new cross sections for that interval, using a three-point Lagrangian interpolator. The neutronic equations then had new cross sections for the next time step, on either side of the mesh point. The finite difference form of the heat transport equation was collected into the more familiar tri-diagonal matrix, and the temperature profile was updated using the same forward-elimination, backward-substitution method.

RESULTS

The transient was initiated, once the steady state was found, by increasing the core debris height (according to the user-input mass accumulation rate) with time. Several input parameters were varied, including fuel debris accumulation rate, initial fuel debris temperature at critical, and the temperature at which the support cylinder failed. This failure was driven by the radial-heat-transfer model, which predicted the cylinder wall temperature with time. When the support structure failed, the core debris column started a downward acceleration (driven by gravity, but also retarded by buoyancy), causing neutronic shutdown of the excursion because of increased axial neutron leakage. The best estimate for the mass accumulation rate was equal to 100 g/sec,

and the best estimate for the initial fuel debris temperature at critical was 650 K. The best estimate for structural failure of the support cylinder was 908 K.

Table 1 shows the predicted energy release as a function of mass accumulation rate, per fuel debris cylinder, for the base case conditions, where all other input parameters are assumed to be best estimate. Initial fuel debris temperature is equal to 650 K. The transients that are driven with higher reactivity insertion rates result in the higher yields, as expected.

Table 1. Energy Release versus Fuel Debris Accumulation Rate.

dm/dt (g/sec)	Energy Release = $\int P dt$ (MJ)
50	3.616
70	3.941
100	4.357
150	4.962
200	5.481
300	6.378
400	7.144
500	7.861

Table 2 shows the predicted energy release as a function of initial core debris temperature. The fuel debris mass accumulation rate is equal to 100 g/sec. As the starting temperature of the fuel debris increases, less energy is required before the structure fails.

Table 2. Energy Release versus Initial Fuel Debris Temperature.

Initial T_{core} (K)	Energy Release = $\int P dt$ (MJ)
650	4.357
700	3.813
750	3.214
800	2.587
850	1.976
875	1.704
900	1.342

Figure 1 illustrates a plot of average core power as a function of time, for a set of five different mass accumulation rates (100 to 500 g/sec). These mass accumulation rates correspond to increasing reactivity insertion rates.

Figure 1. Average Power vs. Time.
(Comparison of Mass Addition Rate)

Figure 2 shows the variation in total energy release with increasing mass addition rate, and Figure 3 shows the variation in energy release with initial fuel debris temperature. Figure 4 shows the sensitivity of the total energy release to the assumed failure temperature of the outer support structure. If this support structure fails at a higher temperature, the transient is allowed to progress further before shutdown, and total yield is increased. In this particular problem, it was not well understood whether this failure criterion should be taken as the material's melting point, or perhaps another, slightly lower temperature (where structural rigidity was reduced) should be assumed.

FUTURE WORK

The ATHENA code can be extended to a fully two-dimensional, multigroup simulator. The existing code, in addition to the five-diagonal matrix inverter routine, also allows the user to choose successive overrelaxation (SOR), with user-input inner iterations per outer, SOR parameters, convergence criteria, etc. The 2D (r,z) ATHENA code will employ both SOR and an alternating-direction implicit (splitting) algorithm. The energy equation also is being extended to include fluid motion (computational fluid dynamics, using the SIMPLE⁴ algorithm). This simulator will have the capability to explicitly model the coevolving neutronic and fluid dynamic fields that characterize solution critical excursions. Applications include water-reflood reactor accidents, waste tank criticalities, and fuel storage basin criticality accidents that might occur under water.

Figure 2. Yield vs. Mass Addition.
(Initial Fuel Temp = 650 K)

Figure 3. Yield vs. Initial Temp.
(Mass Addition Rate = 100 g/sec)

Figure 4. Yield vs. Failure Criteria.
(Mass Addition Rate = 100 g/sec)

CONCLUSIONS

This paper has presented results from a coupled one-dimensional nuclear kinetics, heat transport simulation of a recriticality in a thermal system. The best estimate for the energy release from this event was on the order 4.4 MJ per lattice unit. When one multiplies this value by the number of such units in the system (600), the total yield for this hypothetical accident scenario was on the order of 2.6 GJ, which is approximately a factor of twenty less than the previously reported⁵ 60 GJ. This earlier result was based on far cruder assumptions.

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LIST OF SYMBOLS

- $B_z(t)$ = axial buckling function
 β = delayed neutron fraction = $\sum_l \beta_l$
 β_l = delayed neutron fraction for delayed group l
 C_l = delayed neutron precursor concentration, group l
 C_p = specific heat
 D_g = neutron diffusion coefficient for group g
 δ = extrapolation distance
 $H(t)$ = height of fuel debris stack
 k = thermal conductivity
 $\nu \Sigma_{f,g}$ = ν -fission cross section for group g
 $\Sigma_{a,g}$ = absorption cross section for group g
 $\Sigma_{R,1}$ = removal cross section for group 1
 $\quad = \Sigma_{a,1} + \Sigma_{1,2}$
 $\Sigma_{1,2}$ = downscatter cross section
 λ_l = delayed neutron precursor decay constant
 $\dot{m}$ = mass addition rate
 ρ = average fuel debris density
 ρ_f = density of molten fuel added to cylinder
 $\phi_g(r, t)$ = neutron flux for group g
 $q(r, t)$ = volumetric heat source density
 $T(r, t)$ = temperature
 R = radius of fuel debris stack
 v_g = neutron velocity for group g

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