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THERMAL CRITICALITY IN A REPOSITORY ENVIRONMENT

by

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ABSTRACT

This report explores a scenario in which burial containers fail and fissile material is transported through the tuff by water to some location, away from the burial site, where an over-moderated critical mass gradually accumulates. Because of the low solubilities of plutonium and uranium, and the low ground water velocities, the analysis shows that such a scenario with ^{239}Pu is probably impossible because the time required to accumulate a critical mass is large compared with the half-life of the ^{239}Pu . In the case of ^{235}U , the analysis indicates that the accumulation rates are so low that relatively small fission power levels would consume the ^{235}U as fast as it accumulates, and that the thermal conductivity of the tuff is large enough to prevent a significant increase in temperature. Thus, the conditions for the removal of water by boiling and the associated autocatalytic increase in reactivity are not met in the case of ^{235}U . An explosive release of energy does not appear to be possible. A simple water voiding model, which allows water removal at about the fastest possible rate, was used to explore a scenario in which the fuel accumulation rate was arbitrarily increased enough to cause water boiling and the associated dryout of the tuff. Calculations for this case indicate that disruption of the tuff, leading to a neutronic shutdown, would probably occur before an explosive energy release could be generated. Additional scenarios, which should be investigated in future work are identified.

I. INTRODUCTION

A recent unpublished report by Bowman and Venneri[1] asserts that over-moderated, critical configurations might form at some future time following the burial of large concentrations of ^{239}Pu or highly enriched uranium. They further assert that the criticality event might lead to boiling of water, and, because of the over-moderation, that the subsequent voiding of water could lead to an autocatalytic increase in reactivity and perhaps to the explosive release of energy. This report explores some of the issues related to the Bowman and Venneri hypothesis. Given the amounts of fissile material to be buried, it is probably not possible to argue that criticality is impossible; in fact the Oklo natural reactors[2] support the assertion that criticality events are possible. The following analysis explores a scenario in which fuel in the form of pure ^{239}Pu or ^{235}U accumulates at some location other than the original burial site as a result of water transport, and eventually builds to a critical mass. Based on estimated water transport velocities, the analysis shows that achievement of such a critical configuration with ^{239}Pu is probably impossible because by the time the critical mass could accumulate (many half-lives for ^{239}Pu), the ^{239}Pu would have decayed to ^{235}U . For the case of ^{235}U , a critical mass might accumulate during a time period short compared to the half-life of ^{235}U , but the power level required to build up a temperature close to the boiling temperature of water would consume the ^{235}U much faster than it could accumulate. Thus, autocatalytic behavior for this particular scenario seems to be physically impossible.

There are other possible scenarios in which an over-moderated criticality event might occur; the scenario just described is perhaps the easiest to analyze. Some of these other scenarios involve criticality with the fuel still at or near its original burial site. With spent fuel, a single container would contain as much as 10 kg of ^{239}Pu and 16 kg of ^{235}U [3]. ANL-5800[4] reports critical masses for reflected spheres of ^{239}Pu as low as 2.5 kg and for reflected spheres of highly enriched uranium as low as 9 kg*. Over moderation may not be an issue for the specific

*ANSI standards for assemblies of these isotopes are 5 kg and 20 kg, respectively, so long as surrounding materials do not cause k_{eff} to increase by more than the increase that would be caused by an infinite water reflector. The appropriate limits for a repository environment were not determined in this study.

configurations described in ANL 5800, but even with spent fuel there is enough fissile material to make a critical configuration if the proper geometrical arrangement can be achieved. Some configurations might be over-moderated. The presence of ^{238}U surely makes criticality with spent fuel difficult, but perhaps not impossible. Criticality might be achieved by the combination of water ingress into and/or around the container, gradual reconfiguration of the fissile material, and preferential leaching and dispersal of poisons away from the fissile material. Reactivity insertion rates for such configurations would almost certainly be low, but perhaps not as low as for the scenario outlined in the first paragraph.

Another possible scenario might involve some geological change which would cause the removal of water after critical or near-critical configuration has formed. An initial, crude look at such a scenario was made by increasing the reactivity insertion rate to a level high enough to cause water boiling and then modeling the subsequent water removal using a preliminary water voiding model. The results suggest that the energy release might be large, but not explosive. This analysis is described in Appendix C.

An additional issue, not explored for the work described here, is the amount of ^{238}U that might accumulate with the fuel. The presence of ^{238}U may act as a poison, but it also provides a mechanism to replace some, perhaps a large fraction, of the ^{239}Pu or ^{235}U consumed during a criticality event. This can impact both the duration of the event and the power levels achieved. The presence of ^{238}U played a significant role in the analysis of the operation of the natural reactors at Oklo.

This report documents the work completed so far. Analysis of other possible criticality scenarios may be considered at some future date.

II. FAR FIELD CRITICALITY

The criticality scenario analyzed here presumes that the integrity of the burial containers is compromised so that fuel (specifically, ^{239}Pu or ^{235}U) is transported away from the burial site and begins to accumulate at some location away from the burial site and eventually forms a critical

mass. The geometrical configuration of the mass is uncertain and will probably be determined by the shapes and distributions of fissures in the tuff at a location where the water chemistry would dictate that the fuel would be deposited in or on the tuff walls forming the flow path. As an idealization, the analysis follows Bowman and Venneri[1] and assumes that the critical mass is spherical in shape, is uniformly distributed in the tuff and water, and that the fuel-bearing tuff is imbedded in an infinite medium of tuff with the same water content as the tuff in the fuel-bearing, spherical region. To estimate accumulation rates, the analysis assumes that water is moving through the tuff with a superficial velocity v . One can then estimate the mass flux of the fuel as (assuming a water density of unity)

$$s v \quad (1)$$

where s is the solubility of the fuel. Next, assume that this mass flux of fuel enters the spherical region where the fuel is to accumulate, but that no fuel leaves the region. Further assume that water enters and leaves the region in such a way that the water content remains constant. One can then estimate the rate of accumulation in a sphere of radius r as

$$\pi r^2 s v . \quad (2)$$

This calculation of the mass accumulation rate admittedly over simplifies the process, but it also very likely maximizes the accumulation rate for given values of s and v .

In determining the reactivity state of the spherical configuration, the presence of fuel in the water outside the sphere was neglected. The tuff configuration was arbitrarily selected to have about 10% porosity, with the porosity half-filled with water. Thus, the water volume fraction was assumed to be 5%. B. Shi performed several VIM calculations of k_{eff} as a function of the mass of fuel M_f in the spherical configuration[5]. These calculations were used to estimate the derivative of the reactivity with respect to mass at the point where criticality is achieved. If one designates this derivative as W_f , then one finds reactivity insertion rate at the time of criticality as

$$R_f = W_f \pi r^2 s v . \quad (3)$$

Designating the critical mass as M_{cf} , one can estimate (neglecting losses due to radioactive decay) the time, t_o , required to achieve criticality as

$$t_o = \frac{M_{cf}}{\pi r^2 s v} . \quad (4)$$

Table 1 shows numerical values for some of the parameters used in the expressions (1) through (4), based in part on Shi's VIM calculations. In the table, β is the delayed neutron fraction. Some of the numbers in the table have large uncertainties. For example, Ref. 3 shows a probability distribution for the water percolation rate that extends up to 5 mm/y with a mean of 1 mm/y. The number 0.2 mm/y is based on calculated results presented elsewhere in the same report. On the other hand, the solubility used for ^{239}Pu is probably about the largest value that can be justified[6]. This parameter depends on temperature and pH and may vary with location in the tuff. The times required to achieve criticality for spherical configurations using ^{239}Pu as fuel are seen to be more than a 1000 times the half-life for ^{239}Pu . Order-of-magnitude changes in either the solubility or the water velocity would not change the conclusion that criticality using ^{239}Pu fuel is impossible unless a much faster mechanism can be identified for accumulating the critical mass; otherwise, by the time the required amount of ^{239}Pu could accumulate, all the ^{239}Pu would have decayed to ^{235}U .

Similar uncertainties hold for the solubility of uranium. The calculations described below indicate that order-of-magnitude increases in either the water velocity or the solubility would still leave a substantial margin between the temperature in the fuel bearing region and the water boiling temperature, but an order of magnitude increase in both quantities could cause the calculated water temperature to approach or, perhaps, exceed the boiling temperature. The VIM calculations indicate that for the 200 cm spherical configuration, removal of the water might not cause a significant increase in the reactivity; but for the 300 cm sphere, water removal probably would cause an increase. Should water removal occur, preliminary calculations shown in Appendix C indicate that super-prompt-critical power excursions probably would not occur. The energy release, however, could significantly disrupt the tuff near the critical configuration.

III. POINT KINETICS EQUATIONS

Power generation in the spherical configuration envisioned in the preceding paragraphs can be modeled using the standard point kinetics equations. These equations are

$$\frac{dP}{dt} = \frac{\beta}{\Lambda} (\rho - 1) P + \sum_i \lambda_i C_i + S , \quad (5)$$

and

$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} P - \lambda_i C_i , \quad (6)$$

where P is the power, t is time, Λ is the prompt neutron lifetime, ρ is the net reactivity in \$, λ_i is the decay constant for the i -th delayed neutron precursor group, C_i is the precursor concentration for the i -th group, S is the external neutron source, and β_i is the fraction of delayed neutrons from the i -th group. For the present analysis, the external neutron source was assumed to be due to spontaneous fissioning of the fuel. One can estimate the source as

$$S \approx \frac{E_f V}{\Lambda v} Z , \quad (7)$$

where E_f is the energy release per fission, V is the volume of the multiplying region, v is the number of neutrons released per fission, and Z is the rate of spontaneous neutron production per unit volume. Making use of (4) and neglecting the loss of fuel as a result of radioactive decay, the rate of accumulation of fuel can be expressed as

$$\pi r^2 s v = \frac{M_{cf}}{t_o} ,$$

and the amount of fuel accumulated at time t would be given by

$$\frac{M_{cf}}{t_o} (t_o + t) .$$

In this expression, $t = 0$ is explicitly chosen to be at a time t_o after the fuel begins to accumulate.

Using this expression, one can now calculate the rate of neutron production per unit volume as

$$Z = \frac{v_s \phi \ln 2 N_a}{A T_{1/2} V} \frac{M_{cf}}{t_o} (t_o + t) ,$$

where ν_s is the number of neutrons released per spontaneous fission, ϕ is the fraction of decays that result in spontaneous fission, N_a is Avogadro's number, A is the atomic mass of the fuel, and $T_{1/2}$ is the half-life of the fuel. Assuming $\nu_s \approx \nu$, one can replace (7) by

$$S \approx \frac{E_f \phi \ln 2 N_a}{\Lambda A T_{1/2}} \frac{M_{cf}}{t_o} (t_o + t) . \quad (8)$$

The most important parameter in (5) is the net reactivity ρ . To evaluate this, one must identify the feedback mechanisms. The present analysis considers three processes, namely, the reactivity change caused by the accumulation of fuel, the reactivity effect of temperature change in the fuel-bearing region, and the reactivity effect of fuel consumption (fission or transmutation of fissile isotopes). Thus, the reactivity can be expressed as

$$\rho = R_f t + \alpha_T (T - T_o) + \alpha_B \int_{-\infty}^t dt' P(t') , \quad (9)$$

where α_T is the temperature coefficient, T is the temperature at time t , and T_o a reference temperature, and α_B is the consumption coefficient. The reactivity insertion rate is given by (3). The present analysis uses the value estimated by Bowman and Venneri of $-10^{-5} \Delta k/k$ per K for the temperature coefficient α_T . For the consumption coefficient, one can use the expression

$$\alpha_B = - W_f \frac{A \Sigma_a}{E_f N_a \Sigma_f} , \quad (10)$$

where W_f was defined in connection with (3), Σ_a is the macroscopic absorption cross section, and Σ_f is the macroscopic fission cross section. The most complicated part of (9) is the evaluation of the temperature. Appendix A describes the evaluation of the temperature difference $T - T_o$ based on the solution of the transient heat conduction equation for a point source of heat in an infinite medium and a simpler calculation based on a heat transfer coefficient derived from the solution of the steady state heat conduction equation for a distributed spherical source in an infinite medium. For most problems, the latter approach seems adequate and greatly simplifies the analysis.

A. Quasistatic Solutions

Direct numerical solution of (5) and (6), supplemented with (9), proves to be relatively easy and straight forward using a standard ordinary differential equation solver such as the GEAR subroutines. However, over much of the time domain of interest, quasistatic solutions are adequate and the results are more instructive than results from numerical solutions. Appendix B compares direct numerical solutions with the quasistatic solutions developed here.

The quasistatic approximation to the solutions of (5) and (6) obtains by setting the time derivatives to zero. Then one obtains from (6)

$$\lambda_i C_i = \frac{\beta_i}{\Lambda} P, \quad (11)$$

and upon substitution of this result into (5),

$$\frac{\beta}{\Lambda} \rho P = -S. \quad (12)$$

During the period when fuel is accumulating, the reactivity is negative and the power is too small to have any significant effect on the temperature. One finds in this case that

$$P = -\frac{\Lambda S}{\beta \rho}. \quad (13)$$

Following the achievement of criticality, the magnitude of the source term in (5) becomes negligible and (12) can be expressed as

$$\rho = 0. \quad (14)$$

As the reactivity approaches zero, there will be a time interval when neither (13) nor (14) are correct. If one needs to know the power during this period, the equations (5) and (6) must be solved directly. Further, (14) is only approached asymptotically as time increases. In the time period immediately following the achievement of criticality, the reactivity oscillates with a small amplitude about zero, and this oscillation leads to oscillations in the power. The oscillations also manifest themselves in the temperature, but for the cases considered here, the temperature oscillations have amplitudes of only fractions of a degree.

Substitution of (9) in (14) yields

$$R_f t + \alpha_T (T - T_o) + \alpha_B \int_{-\infty}^t dt' P(t') = 0. \quad (15)$$

To solve this equation, one must find an expression for the temperature difference in terms of the power level. The differential equation for the temperature difference can be expressed as

$$M_r C_p \frac{d}{dt} (T - T_o) = P - H (T - T_o), \quad (16)$$

where M_r is the mass of material in the spherical region containing the fuel, C_p is the specific heat of the material in the region, and H is the heat transfer coefficient given by Eq. (A-9) in Appendix A. If one solves (15) for the temperature difference, one finds ($\alpha_T \neq 0$)

$$T - T_o = -\frac{R_f}{\alpha_T} t - \frac{\alpha_B}{\alpha_T} \int_{-\infty}^t dt' P(t'). \quad (17)$$

Substituting this result into (16), leads to the equation

$$-M_r C_p \frac{R_f}{\alpha_T} - M_r C_p \frac{\alpha_B}{\alpha_T} P = P + H \frac{R_f}{\alpha_T} t + H \frac{\alpha_B}{\alpha_T} \int_{-\infty}^t dt' P(t'). \quad (18)$$

If in this equation, one defines the energy release as

$$E = \int_{-\infty}^t dt' P(t'), \quad (19)$$

then one obtains the following differential equation for E :

$$-M_r C_p \frac{R_f}{\alpha_T} - M_r C_p \frac{\alpha_B}{\alpha_T} \frac{dE}{dt} = \frac{dE}{dt} + H \frac{R_f}{\alpha_T} t + H \frac{\alpha_B}{\alpha_T} E. \quad (20)$$

One can now define

$$\Gamma = \frac{H \frac{\alpha_B}{\alpha_T}}{M_r C_p \frac{\alpha_B}{\alpha_T} + 1}. \quad (21)$$

Making use of this definition, one can rewrite (20) after considerable rearrangement as

$$\frac{dE}{dt} + \Gamma E = -\frac{R_f \Gamma}{\alpha_B} \left[\frac{M_r C_p}{H} + t \right]. \quad (22)$$

Assuming that $E(0) = 0$, direct substitution demonstrates that the solution to (22) is

$$E = - \frac{R_f}{\alpha_B} \left\{ t - \frac{\alpha_T}{\alpha_B H} [1 - e^{-\Gamma t}] \right\}. \quad (23)$$

From this result, one readily finds the power to be

$$P = - \frac{R_f}{\alpha_B} \left\{ 1 - \frac{\alpha_T \Gamma}{\alpha_B H} e^{-\Gamma t} \right\}, \quad (24)$$

and the expression for the temperature difference to be

$$T - T_o = - \frac{R_f}{\alpha_B H} (1 - e^{-\Gamma t}). \quad (25)$$

In these expressions, both α_T and α_B are negative, but the solutions continue to hold both in the limit $\alpha_T \rightarrow 0$ and for positive values of α_T so long as

$$M_r C_p \frac{\alpha_B}{\alpha_T} + 1 < 0. \quad (26)$$

A special case occurs when $\alpha_B = 0$. One can find the energy release, power, and temperature difference in this case by taking the limits of (23 - 25), but it is easier to solve (15) for the temperature difference. One finds ($\alpha_T < 0$)

$$T - T_o = - \frac{R_f}{\alpha_T} t. \quad (27)$$

Substitution of this result into (16) yields after some rearrangement,

$$P = - M_r C_p \frac{R_f}{\alpha_T} - H \frac{R_f}{\alpha_T} t. \quad (28)$$

The energy release then obtains from the integral of this expression and is found to be

$$E = - M_r C_p \frac{R_f}{\alpha_T} t - H \frac{R_f}{\alpha_T} \frac{t^2}{2}. \quad (29)$$

B. Discussion

The results found in equations (23 - 25) show that for the feedbacks assumed, both the power and the temperature difference approach constant values as time increases and that the

energy release increases linearly with time. Further, the asymptotic solutions do not depend on the temperature coefficient so long as it is negative or satisfies the constraint given by (26) when positive. For situations when criticality depends predominately on thermal neutrons, the fuel consumption reactivity coefficient is given by (10). One finds approximately,

$$\frac{\alpha_B}{W_f} = - 1.43 \times 10^{-14} \frac{\text{kg}}{\text{J}} ,$$

for ^{235}U , and

$$\frac{\alpha_B}{W_f} = - 1.70 \times 10^{-14} \frac{\text{kg}}{\text{J}} ,$$

for ^{239}Pu . Making use of results given in Table 1 for a critical configuration of ^{235}U with radius of 300 cm and a value of 94 W/K for H, one finds for the asymptotic values of the power and temperature change, 90 W and 0.96 K, respectively. For a 200 cm critical configuration of ^{235}U , the corresponding results are (H = 63 W/K in this case) 42 W and 0.67 K, respectively. These results show that unless the water temperature is already essentially at the boiling point, a thermal criticality event under the circumstances postulated will not raise the water temperature significantly and, thus, will not lead to an autocatalytic, prompt critical power excursion.

As noted in one of the introductory paragraphs, one circumstance which could modify the conclusions reached in the preceding paragraph would be the presence of ^{238}U at the site where the ^{235}U was accumulating, or the simultaneous accumulation of ^{238}U and ^{235}U . In this event, the equations developed for the neutron kinetics would have to be augmented by equations accounting for the creation of ^{239}Pu as a result of neutron capture in ^{238}U and its subsequent destruction by fission or neutron capture. Qualitatively, the presence of the ^{238}U would have the effect of reducing the value of α_B in (9). The quasistatic solutions indicate that such a reduction would result in an increase in the asymptotic power and temperature change. It is unlikely that α_B could be made to vanish in this way, but if the reduction were to approach a factor between 50 and 100, the margin between the temperature in the fuel-bearing region and the water boiling temperature might be made to vanish, and the reactivity consequences of water removal would have to be investigated. Note that a higher ^{238}U content might also increase the magnitude of α_T , a help should a fast transient develop. A first step in considering the presence of ^{238}U would be to

perform VIM calculations to quantify the effects of ^{238}U on α_B . This is one avenue of investigation that should be considered in future work on repository criticality problems.

Another scenario might develop out of the one considered above. Suppose that a critical configuration were to occur under the circumstances considered above. As long as fuel continues to be supplied, the configuration might remain essentially at critical for a long time. During this time one might suppose that geological changes occur which cause the amount of water in the tuff to decrease. Presumably, such a decrease would reduce or perhaps stop the accumulation of fuel, but, depending on the rate of decrease, the reactivity increase caused water removal might be greater than the reactivity decrease caused by fuel consumption. Such a scenario should probably be considered in future work on this problem.

Other criticality scenarios, noted in the introductory paragraphs, may be considerably more complicated to analyze than the one considered in this memorandum. These scenarios involve fuel that remains essentially at the burial site, but reconfigures and/or loses neutron poisons and thus becomes critical. Such scenarios may be possible even with spent LWR fuel. Reference 3 indicates that a single burial container may contain as much as 26 kg of fissile material. Depending on how the material is configured and on the amount of neutron absorbers present, this might be enough material to reach criticality. Overmoderation of such configurations cannot, a priori, be ruled out. Investigation of such scenarios should probably begin by looking at work that has already been done on the criticality of spent fuel containers (see for example Ref. 7) to identify the important poisons responsible for maintaining subcriticality. One then needs to investigate the rate at which such poisons might be leached out of the fuel and transported far enough away to cause criticality. Computational tools to model the transport of various chemical species out of the waste package have been developed, but have been applied to radioactive species important to determining the dose at some location outside the repository. It may be necessary to apply these tools to different species than have been analyzed previously in order to estimate the appropriate value of R_f in the quasistatic solutions developed above. If fuel reconfiguration is necessary to achieve criticality, then estimates of reconfiguration rates would also be needed to determine the value of R_f . Estimation of the rate of change of reactivity as "in place" criticality occurs is a second avenue of investigation that needs to be considered in future work on repository criticality.

Either consideration of the presence of ^{238}U or the estimation of reactivity insertion rates for other scenarios might lead to conditions in which temperature changes are large enough that water boiling and removal would have to be considered. In overmoderated situations, the reactivity increase associated with water removal could be large (10's or 100's of \$). Even with substantial amounts of ^{238}U , the value of the temperature coefficient could be such that huge temperature changes would be required to overcome the water voiding reactivity increase. Depending on the details of the voiding process, significant temperature changes might not be possible until most of the water has voided, so high power levels are possible. Some preliminary calculations with very simple water voiding models are described in Appendix C. These calculations indicate that while significant disruption of the tuff in or near the critical configuration might occur, super-prompt-critical power excursions with explosive releases of energy probably would not take place.

IV. CONCLUSIONS

The analysis shows that for a thermal criticality scenario in which fuel accumulates at a location other than the original burial site, the thermal consequences would probably be no more severe than switching on a 100 W light bulb buried somewhere in the repository. Temperature changes less than one Kelvin would be expected. The mildness of the event is due to the very slow accumulation of fissile material caused by the low water velocities in Yucca Mountain tuff and to relative low solubilities for uranium in the water. Because of low solubility and low water velocity, a criticality event involving ^{239}Pu appears to be impossible.

Future work should investigate the impact of fissile material accumulation in the presence of or concurrently with ^{238}U . In addition, the possibility of other scenarios in which critical configurations develop with fissile material at or near the original burial site or in which some geologic mechanism causes water removal from a critical or near-critical configuration should be considered. Some of these scenarios may be more likely to occur than the "far field" scenario considered.

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Table 1. Far Field Criticality Parameters for a Superficial Water Velocity of 0.2 mm/y

		<i>r</i> , cm	
		200	300
²³⁹ Pu	<i>s</i> , g/cm ³	2.4×10^{-7}	2.4×10^{-7}
	<i>M_{cf}</i> , kg	58	174
	<i>W_f</i> , \$/kg	3.59	1.43
	<i>R_f</i> , \$/y	2.2×10^{-6}	1.9×10^{-6}
	<i>t_o</i> , y	9.6×10^7	1.3×10^8
	β	0.0021	0.0021
²³⁵ U	<i>s</i> , g/cm ³	7.4×10^{-6}	7.4×10^{-6}
	<i>M_{cf}</i> , kg	110	325
	<i>W_f</i> , \$/kg	0.80	0.27
	<i>R_f</i> , \$/y	1.5×10^{-5}	1.1×10^{-5}
	<i>t_o</i> , y	5.9×10^6	7.7×10^6
	β	0.0065	0.0065

APPENDIX A

SOLUTIONS TO THE HEAT CONDUCTION EQUATION

The following paragraphs show solutions to the transient and steady-state heat conduction equation. The solutions are all derived for the case of an infinite homogeneous medium. In fact, all the problems of interest are two-region problems in which a spherical region of tuff containing a low concentration of fissile material is surrounded by tuff with no fuel. The concentrations of fissile material are low enough so that the small impact on the thermal physical properties of the tuff can be neglected. The analysis shown in this memorandum assumes that the tuff is porous SiO_2 with the porosity partially filled with water. The values for the thermal conductivity, specific heat, and density for SiO_2 are taken from Ref. 9. Where temperature dependence was indicated, values for a temperature of about 100°C were taken. The values selected for the conductivity was 0.038 W/cm/K (SiO_2 is an anisotropic material. The value chosen is for the most weakly conducting direction.); for the specific heat, 0.84 J/g/K ; and for the density, 2.44 g/cm^3 . For water, values near 100°C were also chosen, namely, 0.0068 W/cm/K for conductivity, 4.22 J/g/K for the specific heat, and 1 g/cm^3 for the density. The water properties were derived from correlations given in Ref. 10. The procedure defined by equation 10.3-84 in the most recent SAS4A documentation[11] was used to estimate a value 0.03 W/cm/K for the conductivity of the tuff with 10% porosity, half-filled with water. The corresponding value for the thermal diffusivity was estimated to be $0.014 \text{ cm}^2/\text{s}$ (the values actually used in the calculations reported here were 0.026 W/cm/K and $0.012 \text{ cm}^2/\text{s}$, respectively).

Transient Heat Conduction

In the reactivity equation (9), the temperature T is the average temperature in the sphere of fuel-bearing rock and T_0 is the initial value of the temperature. T_0 can be assumed to be the same as the temperature of the tuff at an infinite distance from the fuel zone. To estimate the transient temperature in the fuel-bearing rock, the following analysis assumes that all energy is deposited at the center of the spherical fuel zone and estimates the temperature T as the average of the transient temperature over the zone.

A fairly easy way to find the transient temperature field due to a point source of heat is to make use of the transient temperature field due to a plane heat source. Page 76 of Carslaw and Jaeger[8] shows the following solution for the transient heat conduction equation in a semi-infinite solid with a specified heat flux at the surface:

$$V(z, t) = \frac{1}{k} \sqrt{\frac{\alpha}{\pi}} \int_0^t \frac{d\tau}{\sqrt{\tau}} F(t - \tau) \exp\left(-\frac{z^2}{4\alpha\tau}\right),$$

where V is the change in temperature from and assumed spatially uniform initial temperature, z is the distance from the heating surface, t is time, k is the thermal conductivity, α is the thermal diffusivity, and F is the time dependent heating rate per unit area (the specified heat flux). This solution can also be used to express the temperature change in an infinite medium due to a plane located at $z = 0$ with a heating rate per unit area Q if one replaces F by $Q/2$. One then finds for the plane heat source in an infinite medium,

$$V(z, t) = \frac{1}{2k} \sqrt{\frac{\alpha}{\pi}} \int_0^t \frac{d\tau}{\sqrt{\tau}} Q(t - \tau) \exp\left(-\frac{z^2}{4\alpha\tau}\right). \quad (\text{A-1})$$

Now let U be the temperature change as a function of time t at a point distance r from a point source emitting heat at a time dependent rate Q . Again, the initial temperature is assumed to be spatially uniform and U represents the change from the uniform temperature. Because the transient heat conduction equation is linear, the plane heat source temperature field can be constructed as a superposition of the temperature fields due to an infinite array of point heat sources spread out uniformly over the plane $z = 0$ such that for any area A , the heating rate is AQ . Thus, using a cylindrical system of coordinates, the heat sources in the plane $z = 0$ between ρ and $\rho + d\rho$ and ϕ and $\phi + d\phi$ produce a temperature change at a point z along the axis $\rho = 0$ given by

$$d\rho \rho d\phi U(\sqrt{z^2 + \rho^2}, t),$$

and the temperature change due to all sources in the plane is given by

$$\int_0^\infty d\rho \rho \int_0^{2\pi} d\phi U(\sqrt{z^2 + \rho^2}, t) = 2\pi \int_0^\infty d\rho \rho U(\sqrt{z^2 + \rho^2}, t).$$

But one can write

$$r^2 = \rho^2 + z^2 \quad \Rightarrow \quad r \, dr = \rho \, d\rho ,$$

and making this variable change in the integral on the right hand side and setting this quantity equal to the temperature change given in (A-1), one finds

$$V (z , t) = 2 \pi \int_z^\infty dr \, r \, U (r , t) . \quad (A-2)$$

From this result, one finds

$$U (z , t) = - \frac{1}{2 \pi z} \frac{\partial}{\partial z} V (z , t) . \quad (A-3)$$

Substituting (A-1) into the right hand side of this expression and carrying out the indicated differentiation yields

$$U (r , t) = \frac{1}{16 \pi \sqrt{\alpha} k} \frac{2}{\sqrt{\pi}} \int_0^t d\tau \, \tau^{-\frac{3}{2}} Q (t - \tau) \exp \left(- \frac{r^2}{4 \alpha \tau} \right) . \quad (A-4)$$

The integral must be evaluated numerically. A more convenient variable of integration was found to be

$$u = \frac{r}{2 \sqrt{\alpha \tau}} \quad \Rightarrow \quad du = - \frac{r}{4 \sqrt{\alpha}} \tau^{-\frac{3}{2}} d\tau .$$

With this change of variable, (A-4) can be rewritten as

$$U (r , t) = \frac{1}{4 \pi r k} \frac{2}{\sqrt{\pi}} \int_{u_o}^\infty du \, Q \left(t - \frac{r^2}{4 \alpha u^2} \right) e^{-u^2} , \quad (A-5)$$

where u_o is given by

$$u_o = \frac{r}{2 \sqrt{\alpha t}} .$$

One can readily show that this result satisfies the transient heat conduction equation and that

$$\lim_{r \rightarrow 0} \left[- 4 \pi k r^2 \frac{\partial}{\partial r} U (r , t) \right] = Q (t) .$$

The average temperature change in a sphere of radius R is defined by

$$\bar{U} (R , t) = \frac{3}{R^3} \int_0^R dr \, r^2 U (r , t) .$$

Substitution of (A-5) yields after some manipulation

$$\bar{U} (R , t) = \frac{3 \alpha}{4 \pi R^3 k} \left[W (t) - \frac{4}{\sqrt{\pi}} \int_{u_1}^{\infty} du u^2 W \left(t - \frac{R^2}{4 \alpha u^2} \right) e^{-u^2} \right], \quad (A-6)$$

where

$$W (t) = \int_0^t d\tau Q (\tau) ,$$

and

$$u_1 = \frac{R}{2 \sqrt{\alpha t}} .$$

Examination of (A-6) reveals that the first term in square brackets is the total energy deposited in the sphere while the integral represents the energy removed from the sphere as a result of conduction.

Steady-State Heat Conduction

The integral term in (A-6) complicates both the transient and the quasistatic solution of the kinetics equations. Nevertheless, a few transient solutions were carried out in which the integral was evaluated as needed. Such solutions were used primarily to show that the heat rejection could be adequately represented using a heat transfer coefficient based on the steady-state solution to the heat conduction equation. The steady-state heat conduction equation can be written as

$$\begin{aligned} - \frac{k}{r^2} \frac{d}{dr} r^2 \frac{dT}{dr} &= \frac{3}{4 \pi R^3} Q , & r \leq R ; \\ - \frac{k}{r^2} \frac{d}{dr} r^2 \frac{dT}{dr} &= 0 , & r > R ; \end{aligned} \quad (A-7)$$

where R is the radius of the heated region and Q is the total heating rate. The solutions to these equations are readily found to be

$$T(r) = T(R) + \frac{1}{8 \pi k R^3} (R^2 - r^2) Q, \quad r \leq R; \quad (A-8)$$

$$T(r) = \frac{Q}{4 \pi k r} + T_o, \quad r > R;$$

where T_o is the temperature at an infinite distance away from the heated sphere. Using the first of these solutions, the average temperature in the sphere can be found as

$$\bar{T} = \frac{3}{R^3} \int_0^R dr r^2 T(r) = \frac{Q}{20 \pi k R} + T(R).$$

Using the second solution in (A-8) to evaluate $T(R)$ and substituting into the expression for the average temperature, one then finds

$$\bar{T} = \frac{3 Q}{10 \pi k R} + T_o.$$

Solving this expression for Q ,

$$Q = \frac{10 \pi k R}{3} (\bar{T} - T_o) = H (\bar{T} - T_o).$$

where the heat transfer coefficient H is given by

$$H = \frac{10 \pi k R}{3}. \quad (A-9)$$

APPENDIX B

COMPARISON OF QUASISTATIC AND NUMERICAL SOLUTIONS TO THE KINETICS EQUATIONS

Direct numerical solution to the point kinetics equations (5) and (6) generally confirm the quasistatic solutions, but show transient effects that cannot be seen by consideration of the quasistatic solutions alone. For example, there is a tendency toward damped oscillatory behavior when criticality is first reached. This behavior cannot be predicted by the quasistatic solutions because it originates during the transition period when neither (13) or (14) hold. To illustrate the departure from the quasistatic solutions, the following paragraphs consider two problems in which fuel consumption reactivity effects are neglected. In these cases, the quasistatic solutions after the accumulation of a critical mass are given by (27 - 29). In the first problem, a critical mass of ^{239}Pu is assumed to collect in a spherical tuff volume with radius 200 cm within a time frame of 1000 years. No credible process which leads to such a scenario has been found. In the second, a critical mass of ^{235}U collects in a tuff volume of 300 cm over a time period of nearly 8 million years. This is the scenario considered in the main body of this memorandum. In both cases, the tuff is assumed to have 10% porosity, half-filled with water.

200 cm Sphere of ^{239}Pu

The critical mass for this configuration is shown in Table 1 to be 58 kg. Setting t_o to 1000 years, one finds $R_f = 0.21$ \$/y. Note that if this scenario could be achieved, then one would find $\alpha_B = 5.1 \times 10^{-14}$ \$/J, and substituting these results into (24), one would find the asymptotic power to be 130 kW (note, 3.16×10^7 s/y). Evaluating the heat transfer coefficient H using (A-9), one finds $H = 63$ W/K, and substituting into (25), one finds the asymptotic temperature change to be 2100 K, much more than required to reach the nominal water boiling temperature.

The quasistatic solutions (23 - 25) do not depend on the neutron source strength estimated by (8), but for a direct numerical integration of the kinetics equations, a value for the source must be assumed. Evaluating (8) for ^{239}Pu ($\phi = 3.1 \times 10^{-12}$, $T_{1/2} = 24000$ y) and assuming $\Lambda = 10^{-4}$ s, one

finds $S = 4.2 (t_o + t)$ W/y. Integration of the kinetics equations was carried out with initial conditions

$$\begin{aligned} P(-t_o) &= 0, \\ C_i(-t_o) &= 0. \end{aligned} \tag{B-1}$$

The delayed neutron constants used in the calculation are taken from Keepin[12] and are listed in Table B1.

The plot in Fig. B1 compares the quasistatic solutions for the power and the energy release evaluated using (28 - 29) with the corresponding results obtained by the direct numerical solution of (5 - 6). As already noted, the coefficient α_B in (9) was set to zero for this calculation. The temperature difference in (9) was evaluated by substituting (A-6) for $(T - T_o)$, and using the sum of the fission power and the power generated by the radioactive decay of ^{239}Pu in place of the function $Q(t)$ in the definition of $W(t)$. In showing the quasistatic results, the power during the period between $t = 0$ and the time when $\rho = 0$, was arbitrarily estimated as the larger of the power evaluated using (13) and the power calculated with (26). The reactivity does not reach zero until after $t = 0$ because of the slight amount of heating due to the decay of ^{239}Pu . The numerical solution shows that the power develops oscillations after criticality is achieved. The oscillations are caused by a slight overshoot of the reactivity and initially have a period between 3.5 and 4 days. The period decreases with increasing time, and the amplitude of the oscillations appears to be damped.

Neither the power nor the energy release agree particularly well during the period immediately after the achievement of criticality because of the inability of the quasistatic solution to represent the transition from subcriticality to criticality. Toward the end of the time period shown, there is much better agreement between the quasistatic and numerical energy release solutions. Perfect agreement, even in the longer, term would not be expected because of the different heat transfer models used in the calculations. The heat transfer model represented by (A-6) deposits all energy at the center of the spherical, fuel-bearing region. This will tend to delay conduction of energy out of the region causing a given increase in temperature to suppress the power in the numerical solution relative to the quasistatic solution.

The plot in Fig. B2 compares the quasistatic solution with a direct numerical integration of the kinetics equations, but with the heat transfer model based on the heat transfer coefficient given by (A-9) used in both the quasistatic and the numerical solutions. In this case, a detailed numerical integration of the differential equation in (16) is carried out simultaneously with the numerical integration of (5 - 6). Agreement between the two solutions is improved in this case. More interesting is the comparison of the numerical solutions with the two heat transfer models. Both the solution with the detailed heat transfer model (A-6) and the solution with the simplified model using the heat transfer coefficient in (A-9) exhibit oscillatory behavior in the time period immediately following initial criticality, and the initial period of the oscillations is about the same. However, the oscillations damp much more rapidly in solution with the heat transfer coefficient.

Use of the detailed model (A-6) is very time consuming because the integral has to be evaluated from scratch each time the time step advances. Thus, from a computing standpoint, using the heat transfer coefficient method is preferable. The plot shown in Fig. B3 shows that for most situations, use of the heat transfer coefficient method is acceptable. The plot shows the temperature change as computed using the three methods. The quasistatic solution is considerably lower over the first 0.07 y because (27) neglects the decay heating which causes the first 3 K temperature increase in the numerical solutions. The oscillatory behavior of the power causes relatively small oscillations in the temperature. Further, after the first 0.07 y, the temperature change calculated by the quasistatic method agrees very well with the temperature changes calculated in the two numerical solutions.

300 cm Sphere of ^{235}U

This case is probably much more realistic than the ^{239}Pu case just considered. The reactivity insertion rate and temperature coefficient needed for the numerical integration of (5 - 6) are described in the main part of this memorandum. The neutron source strength was evaluated using the parameters for ^{235}U , $\phi = 7 \times 10^{-11}$ and $T_{1/2} = 7.04 \times 10^8$ y. With $\Lambda = 10^{-4}$ s, one finds from (8), $S = 2.39 \times 10^{-6} (t + t_0)$.

Fig. B1. Comparison of Quasistatic and Numerical Solutions for the Power and Energy Release with ^{239}Pu Fuel Using Detailed Heat Transfer Model in the Numerical Solution.

Fig. B2. Comparison of Quasistatic and Numerical Solutions for the Power and Energy Release with ^{239}Pu Fuel Using Heat Transfer Coefficient Model in the Numerical Solution.

Fig. B3. Comparison of Quasistatic and Numerical Solutions for the Temperature Change with ^{239}Pu Fuel.

Fig. B4. Comparison of Quasistatic and Numerical Solutions for the Power and Energy Release with ^{235}U Fuel Using Detailed Heat Transfer Model in the Numerical Solution.

Fig. B5. Comparison of Quasistatic and Numerical Solutions for the Power and Energy Release with ^{235}U Fuel Using Heat Transfer Coefficient Model in the Numerical Solution.

Fig. B6. Comparison of Quasistatic and Numerical Solutions for the Temperature Change with ^{235}U Fuel.

APPENDIX C

WATER VOIDING

The paragraphs which follow develop two crude models for describing the removal of water from a critical configuration in the event that the water temperature reaches the boiling temperature. The models represent two extremes of the possible range of water behavior in the tuff environment. In the first model, water vapor can move freely out of the fuel-bearing region and carries no liquid with it. In this case, water is removed at exactly the rate at which it vaporizes. In the second model, liquid can move freely, but the liquid prevents the escape of vapor. The model further assumes that all vapor is formed at the inner edge of the liquid/vapor interface with the vapor contained in a spherical bubble whose center coincides with the center of the spherical fuel-bearing region. In both models, the water vaporizes at nominal atmospheric pressure. Because liquid or vapor are assumed to move freely, there is no buildup of water vapor pressure at any time. In both models, the rate of vapor formation is determined by the heating rate P_{net} and the latent heat of vaporization for water λ_w so that the rate of change of water vapor mass m_v can be expressed as

$$\frac{dm_v}{dt} = \frac{P_{net}}{\lambda_w} . \quad (C-1)$$

Reference 10 indicates that $\lambda_w = 2.3 \times 10^6$ J/kg.

Free Vapor Model

The heating rate in (C-1), once the boiling temperature is reached, can be expressed as

$$P_{net} = P - H (T_b - T_o) ,$$

where P is the fission power, H is the heat transfer coefficient (Eq. (A-9)), T_b is the boiling temperature, and T_o is the ambient reference temperature. Substituting into (C-1) and integrating with respect to time, one finds

$$m_v = \frac{1}{\lambda_w} \int_0^t dt' P (t') - \frac{H}{\lambda_w} (T_b - T_o) t , \quad (C-2)$$

where $t = 0$ corresponds to the time when boiling begins. The equation assumes no vapor mass prior to boiling. If one defines M_w to be the total water mass in the fuel-bearing region and W_w to be the reactivity change caused by removing all water, then the reactivity effect of vaporizing the mass m_v can be expressed as

$$\rho_v = \frac{W_w m_v}{M_w} = \frac{W_w}{M_w \lambda_w} \int_0^t dt' P (t') - \frac{W_w H}{M_w \lambda_w} (T_b - T_o) t . \quad (C-3)$$

This term must be added to the right-hand-side of (9). One then finds, after some rearrangement,

$$\begin{aligned} \rho = & R_f t + \alpha_T (T_b - T_o) + \alpha_B \int_{-\infty}^0 dt' P (t') \\ & + (\alpha_B + \frac{W_w}{M_w \lambda_w}) \int_0^t dt' P (t') - \frac{W_w H}{M_w \lambda_w} (T_b - T_o) t . \end{aligned} \quad (C-4)$$

In this expression, as in (C-2) and (C-3), $t = 0$ is the time when boiling begins. Using the quasistatic approximation (14) and noting that

$$\alpha_T (T_b - T_o) + \alpha_B \int_{-\infty}^0 dt' P (t') = 0 ,$$

one can solve this expression for the integral of the power to find

$$\int_0^t dt' P (t') = - \frac{R_f t - \frac{W_w H}{M_w \lambda_w} (T_b - T_o) t}{\alpha_B + \frac{W_w}{M_w \lambda_w}} . \quad (C-5)$$

The power obtains by differentiation of this expression with respect to time:

$$P = - \frac{R_f - \frac{W_w H}{M_w \lambda_w} (T_b - T_o)}{\alpha_B + \frac{W_w}{M_w \lambda_w}} . \quad (C-6)$$

It is somewhat easier to interpret this result if one rewrites it in the form

$$R_f + \alpha_B P + \frac{W_w}{M_w \lambda_w} [P - H (T_b - T_o)] = 0 .$$

From this result, keeping in mind that $\alpha_B < 0$, it is clear that the power tries to seek a level such that the sum of the reactivity insertion and the reactivity contribution from water voiding are exactly balanced by fuel consumption. Such a power level can be found if the numerator in (C-6) is negative and the denominator is positive, or when the numerator is positive and the denominator is negative. There is no particular reason to believe that the fission power would have this value prior to the onset of water boiling, so there would likely be transient effects which this quasistatic solution would fail to track.

For the ^{235}U configuration considered in Section III.B of this report, Shi[5] found the reactivity worth for water removal to be about 3 \$, and for a corresponding configuration of ^{239}Pu , about 11 \$. For the calculations which follow, the higher of these values will be used. For the conditions described, M_w has the approximate value 5700 kg. One then finds

$$\frac{W_w}{M_w \lambda_w} \approx 8.4 \times 10^{-10} \frac{\$}{\text{J}} \quad \text{and} \quad \frac{W_w H}{M_w \lambda_w} \approx 2.5 \frac{\$}{\text{y} \cdot \text{K}} . \quad (\text{C-7})$$

From the calculations described in Section III.B, it is apparent that boiling temperatures would be reached (assuming a temperature change of about 80 K) if the reactivity insertion rate in Table 1 were increased by a factor of 100. Putting this value along with the values in (C-7) into (C-6), one finds that the numerator is negative and the denominator positive. The steady state power level would be approximately 7.5 kW.

Free Liquid Model

In this model, the fuel-bearing region is divided into two zones. In the inner zone, water exists only in the form of vapor, while in the outer zone, water exists only in liquid form. For a given mass m_v of vapor, the volume of the vapor zone can be expressed as

$$\frac{m_v R_w T}{P_b} ,$$

where R_w is the specific gas constant, T is the vapor temperature (assumed to be the same as the tuff temperature in the vapor zone), and P_b is the pressure at which boiling occurs (assumed constant). The water vapor is assumed to obey the ideal gas law. With this result, the vapor volume fraction can be expressed as

$$\frac{m_v R_w T}{V_t P_b},$$

where V_t is the total volume of the fuel-bearing region. All vapor is produced as a result of heating in the liquid region. Neglecting spatial variations in the power, the net heating rate in the liquid region can be expressed as

$$P_{net}^l = \left[1 - \frac{m_v R_w T}{V_t P_b} \right] \left[P - H (\bar{T} - T_o) \right],$$

where $\bar{T}$ is the average temperature in the fuel bearing region. The average temperature will be defined later. Substituting this result into (C-1), one finds the following expression for the rate of change of the vapor mass:

$$\frac{dm_v}{dt} = \frac{1}{\lambda_w} \left[1 - \frac{m_v R_w T}{V_t P_b} \right] \left[P - H (\bar{T} - T_o) \right]. \quad (C-8)$$

If one neglects the heat capacity of the water vapor, then the enthalpy of the tuff in the vapor region can be expressed as the product of the volume of the region, the density of the region, and the specific enthalpy of the tuff. This product may be written as

$$\rho_r \frac{m_v R_w T}{P_b} h,$$

where ρ_r is the density and h is the specific enthalpy of the tuff. The change in this expression in time dt can be expressed as

$$\rho_r \frac{R_w}{P_b} \left[m_v T \frac{dh}{dt} + m_v h \frac{dT}{dt} + T h \frac{dm_v}{dt} \right] dt.$$

Contributors to this change are heating in the vapor zone and the addition of tuff to the vapor zone as the volume of the zone expands. Thus,

$$\rho_r \frac{R_w}{P_b} \left[m_v T \frac{dh}{dt} + m_v h \frac{dT}{dt} + T h \frac{dm_v}{dt} \right] dt = \left\{ \frac{m_v R_v T}{V_t P_b} \left[P - H (\bar{T} - T_o) \right] + \rho_r h_b \frac{R_w T}{P_b} \frac{dm_v}{dt} \right\} dt .$$

Canceling the common factor of dt and rearranging leads to the result

$$\rho_r \frac{R_w}{P_b} \left[m_v T \frac{dh}{dt} + m_v h \frac{dT}{dt} \right] = \left\{ \frac{m_v R_v T}{V_t P_b} \left[P - H (\bar{T} - T_o) \right] + \rho_r (h_b - h) \frac{R_w T}{P_b} \frac{dm_v}{dt} \right\} \quad (C-9)$$

If one assumes a temperature independent specific heat, then the enthalpy can be expressed as

$$h = \int_0^T dT' C_p^r (T') = C_p^r T ,$$

where C_p^r is the specific heat and (C-9) can be written as

$$2 \rho_r \frac{R_w}{P_b} m_v C_p^r T \frac{dT}{dt} = \left\{ \frac{m_v R_v T}{V_t P_b} \left[P - H (\bar{T} - T_o) \right] + \rho_r C_p^r (T_b - T) \frac{R_w T}{P_b} \frac{dm_v}{dt} \right\}$$

Canceling common factors and rearranging, this becomes

$$\frac{dT}{dt} = \frac{P - H (\bar{T} - T_o)}{2 V_t \rho_r C_p^r} + \frac{T_b - T}{2 m_v} \frac{dm_v}{dt} . \quad (C-10)$$

Equations (C-8) and (C-10) are to be solved with the initial conditions $m_v = 0$ and $T = T_b$, and they must be coupled with the kinetics equations (5) and (6). The term

$$\rho_v = \frac{W_w m_v R_w T}{V_t P_b} ,$$

must be added to the right-hand-side of the reactivity equation (9) to account for the reactivity change caused by vapor generation. Also in (9), the temperature T should be replaced by the average temperature, defined as

$$\bar{T} = \frac{\rho_{rw} V_t T_b + (\rho_r T - \rho_{rw} T_b) \frac{m_v R_w T}{P_b}}{\rho_{rw} V_t + (\rho_r - \rho_{rw}) \frac{m_v R_w T}{P_b}}, \quad (C-11)$$

where ρ_{rw} is the density of tuff with the water in the porosity.

With the initial conditions specified, the coefficient of the second term on the right-hand-side of (C-10) goes to the indeterminate form 0/0 when the time t approaches the time for the onset of boiling t_b . However, if one assumes that the indeterminate form has a finite value, then one finds that

$$T - T_b \approx \left(\frac{dT}{dt} \right)_b (t - t_b) \quad \text{and} \quad m_v \approx \left(\frac{dm_v}{dt} \right)_b (t - t_b)$$

when t is greater than but sufficiently close to t_b . The subscript b in these expressions means evaluation at time t_b . If one substitutes these results into (C-10) and takes the limit as t approaches t_b , then one can solve for the derivative of the temperature at time t_b to find

$$\left(\frac{dT}{dt} \right)_b = \frac{P - H (T_b - T_o)}{3 V_t \rho_r C_p'}.$$

A test calculation using the Free Liquid Model was performed using the 3-m sphere considered in Section III.B of this memorandum, but with the reactivity insertion rate arbitrarily increased by a factor of 100 over the value estimated in Table 1. Thus, the subcritical source multiplication portion of the calculation lasted for a period of 7.7×10^4 years. For convenience, changes in the thermo-physical properties of the tuff caused by the removal of water were neglected. Assuming a far-field temperature of about 287 K, once criticality was achieved, almost an additional 210 years were required to bring the temperature up to 373 K, the nominal boiling temperature for water. As considered earlier in this Appendix, the reactivity effect of complete removal of water from the fuel-bearing zone was assumed to be 11 \$. The plot shown in Fig. C1 shows the power and energy release following the onset of boiling. Initially, the mass of water vapor increases slowly, and the corresponding increase in the volume of the vapor region causes a gradual rise in the void reactivity feedback. The net reactivity at the time when boiling begins is computed to be about 10^{-8} \$, and during the first 120 days, it increases to a peak at 17 days of

about 9×10^{-6} \$, decreases to a minimum at 45 days of about -6×10^{-6} \$, increases to a second peak at 82 days of 7×10^{-6} \$, and decreases to a second minimum at 100 days of about 4×10^{-6} \$. By 100 days, the water voiding feedback has increased to about 2.4×10^{-4} \$ and the power level has increased to 37 kW. From this point on, the voiding feedback begins to increase more rapidly. The average rate of increase between 100 and 120 days is about 0.009 \$/y, a value that is nearly a factor of 10 larger than driving reactivity prior to the onset of boiling. After 120 days, the power reaches a peak of 5 GW, a level somewhat higher than the thermal power level of a modern power reactor. The power decreases after this time, primarily because of temperature feedback caused by the heating of the fuel in the vapor region.

Figure C2 shows the temperature for a 9-hour period starting about 122 days after the onset of boiling. The plot in Fig. C3 shows the power and the accumulated energy release during the same period. Some key melting and vaporization temperatures are indicated on the temperature plot. The tuff melting and vaporization temperatures are assumed to be the same as for SiO_2 . The plot shows that more than half an hour before the power peak occurs, some important events occur that could have a significant effect on the reactivity feedback. The feedbacks from these events are not included in the modeling at present. Tuff heating and melting would probably imply significant expansion of the vapor zone, and for the configuration considered, this expansion would almost certainly cause negative reactivity feedback. Thus, the calculation shown is overly pessimistic regarding the power levels that could be reached. Over the last few hours of the transient shown, the water voiding reactivity increases at an average rate of about 0.85 \$/day. The highest net reactivity achieved is only about 0.026 \$. Thus, even with the relatively pessimistic model considered here, a super-prompt-critical power excursion does not occur. The energy release could be very disruptive to the region where the critical configuration is located, but the release is not explosive.

Some one-group, infinite medium calculations[13] indicated that water voiding worths might be as high as 100's of \$ under some circumstances. These calculations may be misleading because they do not account for spectral changes that might occur as the water content changes, but to get an idea what such high void worths might imply, a second calculation was performed in which the water void worth was arbitrarily increased by a factor of 10. All other conditions

were the same as in the previous calculation. In this second calculation, a super-prompt-critical excursion did occur, but all the melting and vaporization temperatures indicated in Fig. C-2 were reached before prompt critical was achieved. If the feedbacks from these phase changes were included in the calculation, there is a good chance that a prompt critical excursion would be avoided in this case also.

Fig. C1. Power and Energy Release as Function of Time after the Onset of Boiling.

Fig. C2. Temperature During 9-Hour Period Starting about 122 Days after the Onset of Boiling.

Fig. C3. Power and Energy Release During 9-Hour Period Starting about 122 Days after the Onset of Boiling.

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