PREDICTION OF MINIMUM UO_2 PARTICLE SIZE BASED ON
THERMAL STRESS INITIATED FRACTURE MODEL

by

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ABSTRACT

An analytic study was employed to determine the minimum UO_2 particle size that could survive fragmentation induced by thermal stresses in a UO_2 -Na Fuel Coolant Interaction (FCI). A brittle fracture mechanics approach was the basis of the study whereby stress intensity factors K_I were compared to the fracture toughness K_{IC} to determine if the particle could fracture. Solid and liquid UO_2 droplets were considered each with two possible interface contact conditions; perfect wetting by the sodium or a finite heat transfer coefficient. This analysis indicated that particles below the range of 50 microns in radius could survive a UO_2 -Na fuel coolant interaction under the most severe temperature conditions without thermal stress fragmentation.

Environmental conditions of the fuel-coolant interaction were varied to determine the effects upon K_I and possible fragmentation. The underlying assumptions of the analysis were investigated in light of the analytic results.

It was concluded that this analytic study seemed to verify the experimental observations as to the range of the minimum particle size due to thermal stress fragmentation by FCI. However the method used when the results are viewed in light of the basic assumptions indicate that the analysis is crude at best, and can be viewed as only a rough order of magnitude analysis. The basic complexities in fracture mechanics make further investigation in this area interesting but not necessarily fruitful for the immediate future.

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NOMENCLATURE

a	= position of the solidification front (radial)
A	= surface area
Bi	= (hR/k) = Biot number (nondimensional)
c	= crack length
c_p	= specific heat
E	= modulus of elasticity
E_n	= energy
h	= surface heat transfer coefficient
k	= thermal conductivity (k_s -solid fuel material, k_c -coolant material)
K	= bulk modulus
K_I	= stress intensity factor
K_{IC}	= critical stress intensity factor (fracture toughness)
K_{IP}	= stress intensity factor due to pressure stresses
K_{IT}	= stress intensity factor due to thermal stresses
L	= latent heat of fusion
m	= mass
P	= pressure in the solidifying droplet
r	= radial position in solidifying shell
R	= external radius of drop
r_y	= radius of plastic zone at the crack tip
$\bar{r}$	= (a/R) = nondimensional solidification front position
$T(r,t)$	= temperature in solidifying shell
$\bar{T}(r,t)$	= $T(r,t) - T_m$

$T(a)$	= temperature at solidification front ($=T_m$)
T_m	= melting point of molten material
T_{cool}	= coolant temperature
T_I	= interface temperature (at $r = R$)
$T_s(t)$	= variable surface temperature (T_I)
t	= time
$\bar{t}$	= $(kT_m t/LR^2)$ = nondimensional time
V	= volume
α	= thermal contraction coefficient
α'	= thermal diffusivity
δ	= vapor layer thickness
ρ	= material density
σ_f	= fracture stress
σ_r	= total radial stress
σ_{rP}	= radial pressure stress
σ_{rt}	= radial thermal stress
σ_t	= total tangential stress
σ_{tP}	= tangential pressure stress
σ_{tt}	= tangential thermal stress
ν	= Poisson's ratio

(Note: a bar over a symbol indicates nondimensionalizing.)

1.0 INTRODUCTION

In the design of reactor systems possible accident situations must be considered and their possible consequences evaluated and designed for. The most severe accident that could possibly occur is a melt down of the reactor core. Although this situation has been shown to be highly improbable it ought to be considered. The accident entails hot molten fuel coming into contact with the colder liquid coolant (fuel-coolant interaction FCI). Although the fission process has ceased, there is a large thermal energy reservoir in the fuel which is released in the interaction and could assume the form of disruptive mechanical work. This type of heat transfer interaction is possible in other mechanical systems, but the toxic radioactivity associated with reactor systems makes this possible accident much more hazardous. Safety analyses of this type of accident focus on two areas: developing design constraints which minimize the probability of such an accident and its effects; prediction of the post-accident behavior to aid in design of reactor systems.

This study is formulated from the latter area of post accident prediction. Specifically, the type of reactor studied is the liquid metal fast breeder reactor (LMFBR) with $\text{UO}_2\text{-PuO}_2$ as the fuel and liquid sodium (Na) as the coolant. In the current study UO_2 is used as the fuel material. The type of accident postulated is some type of reactor power excursion caused by a loss of coolant flow or overpower transient. This results in fuel rod failures over a large area of the core and results in molten fuel being dispersed into the sodium

coolant. The energetic consequences of the FCI is not precisely known at this time, but there are theories as to the sequence of events which occur. Some existing mathematical models have predicted that sizeable amounts of mechanical energy [1] can be derived from the molten fuel thermal energy. For the case of UO_2 dispersed in sodium, these predictions have not been experimentally proven, although for an experiment where sodium was dropped into UO_2 larger mechanical energy conversion rates were obtained [2]. Thus it has been experimentally demonstrated that the mode of contact as well as the thermally energy input must be known to predict the results of a FCI. The interaction is thought to yield vapor production at a rapid enough rate to result in an immediate pressurization of the local sodium and a shock wave acting as a piston on the surrounding colder liquid sodium coolant. To produce sodium vapor at this rapid rate either the thermal heat flux must be large or the area of heat transfer from the fuel to the coolant must be increased quickly. Although there are many scenarios presented as to the way the FCI proceeds, there are basically two general theories which follow the aforementioned alternatives.

One can be classified as the spontaneous nucleation theory [3]. In this mechanism perfect liquid-liquid contact and a lack of nucleation sites is assumed. This allows the sodium at the interface with the fuel to heat up beyond its saturation temperature to superheat temperatures which correspond to spontaneous nucleation. The expected results are extremely high pressure pulses due to the rapid generation of the sodium vapor. This method of vapor production

cannot happen when UO_2 is dispersed in sodium because the temperature of the sodium coolant surrounding the UO_2 droplet remains below the spontaneous nucleation temperature of sodium.

The other supposed mechanism for rapid vapor production can be classified as the fragmentation theory. The fuel when immersed in the colder sodium coolant begins to solidify. One possible mechanism for fragmentation is that the solidification process breaks up the UO_2 into numerous smaller pieces. Thus the area available for heat transfer increases rapidly, consequently resulting in more thermal energy released to the fuel in a short span of time. This current work is based upon this latter theory of fragmentation.

This fragmentation has been observed experimentally, and it has resulted in pressurizations of a small magnitude. Some mathematical models have shown [5][6] that when constrained to a small volume of sodium the potential mechanical energy output could be great. The process as depicted is very complex, and at this time some aspects of it have been investigated. The mode of contact between fuel and coolant, and the rate of area generation of the fuel as time proceeds are two areas where parametric investigations have been done [6]. Specifically, the mechanism for fragmentation of the UO_2 fuel is thought to be by the thermal stresses generated as the fuel solidifies.

This current study is based upon an extension of the thermal stress model and a fracture mechanics approach to the fragmentation mechanism. The first objective is to determine the minimum UO_2 particle size that could survive thermal stresses induced by sudden cooling in sodium. This analysis is accomplished for initially solid

and liquid particles with two types of interface conditions: perfect solid-liquid interface contact and a finite heat transfer coefficient. The second objective of this study is an evaluation of the results in light of the limiting assumptions of the analysis. More specifically, in the area of fracture mechanics the assumptions made are significant and reviewed in conjunction with the results.

This analysis is based to a large extent on existing experimental works and analytical models. Results from this work hopefully will aid in depicting a possible mechanism consistent with experimental findings of fuel-coolant interactions. At present the complexity of this phenomenon precludes a comprehensive model for it, but it is hoped that this work will help bridge the gap.

2.0 TEMPERATURE CHARACTERISTICS OF FUEL COOLANT INTERACTION

2.1 Introduction

Essential to the determination of thermal stresses in the fuel particle is the knowledge of the transient temperature distribution. There are two types of particles of interest: liquid and solid. To analyze their behavior during solidification and/or cooling two types of boundary conditions are assumed: constant interface temperature and finite heat transfer coefficient between UO_2 and sodium coolant.

Once the temperature distribution has been determined for these four cases, the thermally induced stresses within the solid portion of the particle can be evaluated. This analysis and the fracture mechanics calculations will be presented in the following chapter.

To view the problem in general the overall physical picture is presented first with the governing mathematical model of the solidification and cooling phenomena. Then each case is examined and the classical solutions to the problems reviewed.

2.2 Overview of Phenomenon

In the event of a meltdown of the LMFBR core the fuel disperses into the sodium coolant. According to the fragmentation theory it then solidifies and fragments into smaller particles both liquid and solid. This mechanism generates area which promotes heat transfer at a rapid rate to the sodium. The fuel is assumed to be

in the shape of a sphere (Fig. 2.1) to determine the temperature distribution as a function of time and position. Previous analysis of this phenomenon for initially liquid drops [7] indicated for the liquid drop case that the solidification rate is the limiting process in comparison to the rate of crystal growth in the solid shell. So the objective is to determine the temperature distribution in the solid for both types of drop, as well as the solidification rate for the liquid particle.

The general governing equation obtained by an energy balance for rotationally symmetric temperatures is:

$$\frac{\partial T(r,t)}{\partial t} = \alpha' \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T(r,t)}{\partial r} \right) \quad (2.1)$$

This equation and subsequent analysis is based on the following assumptions:

- 1) Solidification for liquid case is instantaneous [7] in comparison to crystalline growth rate.
- 2) Compressibility is neglected for liquid case.
- 3) Density of both phases of the fuel were taken as the same.
- 4) The transition temperature from liquid to solid UO_2 was taken at a discrete [8] temperature (2800 °C)
- 5) The fission decay heat source in the fuel is neglected.

- 6) Thermal properties were taken as constant in all cases [9].
- 7) The heat transfer coefficient and the interface temperature were both taken as constants when they were alternatively used.

The associated boundary conditions and solutions are discussed for both types of particles.

2.3 Liquid Particle Solidification and Temperature Distribution

For this particular situation a UO_2 liquid droplet is suddenly immersed in an infinite medium of colder liquid sodium. Initially a solid shell forms at the outer boundary of the drop and proceeds to grow toward the center of the drop as the freezing front advances. The boundary conditions for equation (2.1) for this case are

$$T(a, t) = T_m \quad (2.2)$$

$$-k \frac{dT}{dr} \Big|_{r=a} = \rho L \frac{da}{dt} \quad (2.3)$$

$$T(R, t) = T_\infty \quad (2.4)$$

The constant interface temperature corresponds to perfect wetting between the UO_2 and the sodium. The temperature is found by the solution to a solidifying semi infinite body [10], as

$$T_I = \frac{T_H (K_H / \sqrt{\alpha_H'}) + T_C (K_C / \sqrt{\alpha_C'}) \operatorname{erf} \lambda}{(K_H / \sqrt{\alpha_H'}) + (K_C / \sqrt{\alpha_C'}) \operatorname{erf} \lambda} \quad (2.5)$$

where H and C corresponds to the hot and cold materials respectively. The $\operatorname{erf} \lambda$ appears from the condition of a moving solidification front and is evaluated by

$$\left(\frac{C_P T_M}{L \sqrt{\pi'}} \right)_{\text{UD}_2} = \lambda e^{\lambda^2} \left(\frac{K_H \sqrt{\alpha_C'}}{K_C \sqrt{\alpha_H'}} + \operatorname{erf} \lambda \right) \quad (2.6)$$

For the most severe case investigated [9] where the sodium coolant is at 200 °C and the initial fuel temperature $T_m = 2800$ °C, $\lambda = .94$ and T_I is 945 °C. The initial condition is

$$T(r, 0) = T_m \quad (2.7)$$

An approximate solution to the differential equation (2.1) with these boundary conditions was developed by Adams [11]. It is based upon dividing heat flow into the sensible and latent components and solving the differential equation first for latent heat flow and then correcting for the sensible contribution. The temperature distribution is given as,

$$T(r, t) = T_I - \frac{L a^2}{\alpha' C_p} \left(\frac{R-r}{Rr} \right) \frac{da}{dt} + \frac{L a}{C_p \alpha'^2} \left(\frac{R-r}{R-r} \right) \left(\frac{da}{dt} \right)^2 \quad (2.8)$$

$$\times \left(\frac{R}{3} - \frac{r}{6} - \frac{a^2}{2r} + \frac{a^3}{3Rr} \right)$$

and the freezing rate is:

$$\frac{da}{dt} = \frac{2\alpha' c_p (T_m - T_\infty)}{\left(L_m - \frac{L_m^2}{R}\right) \left(1 + \sqrt{1 + \frac{4}{3} \frac{R c_p}{a L} (T_m - T_\infty)}\right)} \quad (2.9)$$

The position of the solid-liquid interface is found by integrating equation (2.9) over the time interval (0 to t).

For the case where there is not perfect wetting between UO_2 and Na caused by either sodium vapor or fission gas release, a heat transfer coefficient (h) is defined. It replaces equation (2.3) and is expressed as:

$$-k_s \frac{dT}{dr} \bigg|_{r=R} = h (T(R,t) - T_{\text{cool}}) \quad (2.10)$$

Two solutions to the equation (2.1) with this new boundary condition were examined by Cronenberg [9]. A numerical solution as developed by Tao was compared to the steady-state approximate solution of London and Seban [12] (see Fig. 2.2). It illustrates for the UO_2 -Na system that the steady state approximation leads to a noticeable error at long times in the solidification rate and position. The analytic steady-state approximation was used in this study for comparative evaluation to the perfect contact condition. It was considered accurate over the short times investigated in this work.

The London and Seban solution is based on the assumption that the internal energy change of the solid with time ($\rho C_p \frac{dT}{dt}$) is small

compared to the energy flow across the solid-liquid interface due to the latent heat of fusion. This results in the fact that the temperature profile remains linear and constant with time although the solid-liquid interface moves toward the center of the sphere. Mathematically the left hand side of (2.1) is set to zero and the equation becomes

$$\frac{d}{dr} \left(r^2 \frac{dT}{dr} \right) = 0 \quad a < r < R \quad (2.11)$$

with the boundary conditions and initial condition given as:

$$T(a, t) = T_M \quad (2.2)$$

$$-K_s \frac{dT}{dr} \Big|_{r=a} = \rho L \frac{da}{dt} \quad (2.4)$$

$$-K_s \frac{dT}{dr} \Big|_{r=R} = h (T(R, t) - T_{\text{cool}}) \quad (2.10)$$

$$T(r, 0) = T_M \quad (2.5)$$

The solution is given as

$$\frac{T(r, t) - T_{\text{cool}}}{T_M - T_{\text{cool}}} = \frac{\left(\frac{a}{R} \right) \left(1 + \frac{r}{R} \left(\frac{1}{Bi} - 1 \right) \right)}{\left(\frac{r}{R} \right) \left(1 + \frac{a}{R} \left(\frac{1}{Bi} - 1 \right) \right)} \quad (2.12)$$

in nondimensional form where Bi is the Biot number (hR/K_s), a relative measure of the surface conductance to the internal shell resistance. Using equation (2.12) in conjunction with (2.4) the time for the solid-liquid interface to move from any position (a) is:

$$t = \frac{LR^2}{h_f T_M} \left(\left(\frac{1 - (r/R)^2}{2} \right) + \left(\frac{1 - (r/R)^3}{3} \right) \left(\frac{1}{Bi} - 1 \right) \right) \quad (2.13)$$

At this point it would be useful to compare the results for the liquid drop solidification for these two different surface boundary conditions. As it will be demonstrated later the size of particles of interest is around 100 microns in radius. Using this as the size for comparison purposes Figs. 2.3 and 2.4 have been constructed. An arbitrary solid-liquid interface position is given to show the general difference in behavior due to the two types of surface boundary conditions. It should be noted that as the heat transfer coefficient increases the rate of solidification increases and the situation approaches the fixed temporary boundary condition. The heat transfer coefficients selected bound the film boiling and nucleate boiling range for the sodium coolant (.1 cal/scm² °C to 41 cal/scm² °C). In Fig. 2.4 the approximation of London and Seban is illustrated resulting in predicted temperatures which underestimate the temperature at a fixed time.

2.4 Solid Particle Temperature Distribution

The origin of the solid particle is assumed to be from a previous fragmentation of a larger initially liquid drop. Although the shapes of these particles vary [4] they are approximated for this analysis by a sphere. Again there are two surface boundary conditions which can be applied, a constant surface temperature (T_I - eqn. 2.3) or a constant heat transfer coefficient (h - eqn. 2.10) and the initial condition equivalent to eqn. 2.5 is $T(r,0) = T_{IN}$ (2.14). Since the particle is solid, B.C. 2.4 does not apply.

The solution to equation (2.1) for the case of the constant surface temperature is given in an infinite series as [13]

$$T(r,t) = T_I + \frac{2R}{r\pi} (T_{IN} - T_I) \left(e^{-pt} \sin \frac{\pi r}{R} - \frac{e^{-4pt}}{2} \right. \\ \left. \times \sin \frac{2\pi r}{R} + \frac{e^{-9pt}}{3} \sin \frac{3\pi r}{R} \dots \right) \quad (2.15)$$

where

$$p = \alpha' \left(\frac{\pi}{R} \right)^2 \quad (2.16)$$

The value of surface temperature, T_I , is taken to be the temperature of the sodium coolant (T_{COOL}). In reality the interface temperature initially (10^{-10} s to 10^{-4} s) can be expressed as approximately the solution to the semi-infinite slab problem for solid, given as

$$T_I = \frac{T_H (K_H / \sqrt{\alpha_H}) + T_C (K_C / \sqrt{\alpha_C})}{(K_H / \sqrt{\alpha_H}) + (K_C / \sqrt{\alpha_C})} \quad (2.17)$$

But as time progresses because the sphere is of finite size and there is no freezing front, T_I decreases asymptotically to T_{COOL} . The final value is assumed in the subsequent analysis. T_{IN} represents the initial temperature of solid particles. In reality the temperature distribution within the sphere is not uniform initially. Since it is assumed to be formed by a previous fragmentation of the solid shell of a liquid drop solidifying, it will have a temperature gradient across its diameter. This situation cannot be handled analytically and it was approximated by this simpler conservative initial condition.

Finally for the case of the fixed heat transfer coefficient the solution is given by Carslaw [13] as

$$T(r,t) = T_{IN} + \frac{3F_0 t}{\rho_s c_p R} + \frac{F_0(5r^2 - 3R^2)}{10K_s} - \frac{2F_0 R^2}{K_s} \sum_{n=1}^{\infty} \frac{\sin \beta_n \frac{r}{R} \exp\left(-\frac{\alpha' \beta_n^2 t}{R^2}\right)}{\beta_n^2 \sin \beta_n} \quad (2.18)$$

where β_n 's satisfy the equation:

$$\tan \beta_n = \beta_n \quad (2.19)$$

and F_0 represents the heat flux from the solid surface as

$$F_0 = h(T_{COOL} - T(R,t)) \quad (2.20)$$

To determine the temperature at the surface $T(R,t)$ r is set equal to R (eqn. 2.18) and $T(R,t)$ is solved for. The result is

$$T(R,t) = \frac{T_{IN} + T_{COOL} \left(\frac{3h}{\rho C_p R} + \frac{Rh}{5Ks} - \frac{2Rh}{Ks} \sum_{n=1}^{\infty} \frac{\exp\left(-\frac{\alpha' E_n^2 t}{R^2}\right)}{\beta_n^2} \right)}{1 + \frac{3h}{\rho C_p R} + \frac{Rh}{5Ks} - \frac{2Rh}{Ks} \sum_{n=1}^{\infty} \frac{\exp\left(-\frac{\alpha' \beta_n^2 t}{R^2}\right)}{\beta_n^2}} \quad (2.21)$$

Both these solutions are approximated by truncating the infinite series. The criterion used to do this is to match the initial condition (2.14) over the solid within 5-10% accuracy. This results in keeping the first five terms in each series solution. As a comparison of these two types of boundary conditions Fig. 2.5 has been constructed to illustrate the general difference between the two surface conditions. It can be seen that as time progresses the surface temperature of the fixed heat transfer coefficient case approaches the sodium coolant temperature.

Now that all the temperature distributions of all four cases have been examined the next objective is the determination of induced stresses within the solid and the prediction of fragmentation by fracture mechanics.

3.0 STRESS GENERATION AND STRESS INTENSITY FACTORS

3.1 Introduction

When the liquid or the solid particle of fuel is immersed in the sodium coolant an uneven temperature distribution is established within the solid portion. Because of this, the cooler, more dense solid material at the surface attempts to contract but is constrained by the hotter less dense interior portion of the solid. This introduces a tensile stress at the surface of the sphere and a compressive stress on the interior. In addition the solid shell of the liquid drop is attempting to contract inward in the radial direction due to these thermal stresses as well as the differential in temperature from its initial state. The liquid core has limited compressibility and the pressure within it rises inducing secondary pressure stresses both radially and tangentially.

If there exists flaws or cracks (a likely occurrence) on the surface of the solid or solidifying liquid, the stresses in that region are intensified. This situation, if the stresses are high enough, can cause the solid to fracture by the crack propagating further into the solid. This is the mechanism of fragmentation induced by non-uniform temperature distributions which has been conceived [7]. Within this chapter the mathematical formulations for these stresses are presented, the fracture mechanics approach is briefly explained and a mathematical model for predicting fracture is presented.

3.2 Stress Generation

The general form of the thermoelastic stress solution for non-uniform temperatures within the solid is solved by Kent [14] and given as

$$\sigma_{rr} = \frac{2\alpha E}{1-\nu} \left[\frac{r^2 - a^2}{r^3(R^3 - a^3)} \int_{C_0}^R \bar{T} r^2 dr - \frac{1}{r^3} \int_{C_0}^r \bar{T} r^2 dr \right] \quad (3.1)$$

$$\sigma_{tt} = \frac{2\alpha E}{1-\nu} \left[\frac{2r^3 + a^3}{2r^3(R^3 - a^3)} \int_{C_0}^R \bar{T} r^2 dr - \frac{1}{r^3} \int_{C_0}^r \bar{T} r^2 dr - \frac{\bar{T}}{2} \right] \quad (3.2)$$

$$\text{where} \quad \bar{T} = T(r, t) - T_m \quad (3.3)$$

and $C_0 = a$ when particle is initially liquid

$= 0$ when particle is initially solid.

In addition the liquid drop by thermal contraction induces an internal pressure in the liquid core and this is given by Cronenberg [9] [15] as

$$P = \frac{6\alpha E}{R^3 + 2a^3 - \nu(4a^3 - R^3) + \frac{2}{3} \frac{E}{K}(R^3 - a^3)} \int_a^R \bar{T} r^2 dr \quad (3.4)$$

where the associated stresses are

$$\sigma_{rp} = \frac{-Pa^3(R^3 - r^3)}{r^3(a^3 - R^3)} \quad (3.5)$$

$$\sigma_{\theta\theta} = \frac{\rho a^3 (2r^3 + R^3)}{2r^3 (a^3 - R^3)} \quad (3.6)$$

These expressions then are utilized with the four different expressions for temperature distributions for each case. For the liquid drop with T_I fixed and the solid drop with h fixed the expressions for $T(r,t)$ are complex so that numerical integration is used to evaluate the stresses. But for the other two cases the expressions are simple enough for evaluation of the stresses analytically. For the initially liquid drop with fixed heat transfer coefficient the tangential stress components are found by substituting equation (2.12) into (3.1) and (3.4) and obtaining

$$\sigma_{\theta\theta} = \frac{2\alpha E (T_M - T_c)}{1-\nu} \left[\frac{(2(\frac{r}{R})^3 + (\frac{a}{R})^3) \left\{ \frac{1}{2} (\frac{r}{R}) - (\frac{a}{R})^3 - \frac{1}{3} (1 - (\frac{a}{R})^3) \right\}}{2 (1 - (\frac{a}{R})^3) (\frac{r}{R})^3 (1 + \frac{a}{R} (\frac{1}{Bi} - 1))} \right. \\ \left. - \frac{1}{2} \frac{(\frac{a}{R} - 1)}{(1 + \frac{a}{R})(\frac{1}{Bi} - 1)} + \frac{1}{2(\frac{r}{R})^3} \left(\frac{\frac{1}{2} (\frac{a}{R}) (\frac{r}{R})^2 - (\frac{a}{R})^2 - \frac{1}{3} (\frac{r}{R})^3 - (\frac{a}{R})^3}{(1 + \frac{a}{R})(\frac{1}{Bi} - 1)} \right) \right] \quad (3.7)$$

$$\sigma_{rr} = \frac{\rho a^3 (2r^3 + R^3)}{2r^3 (a^3 - R^3)} \quad (3.8)$$

$$p = \frac{\alpha E (T_M - T_{cool}) \left[3 \left((\frac{a}{R}) - (\frac{a}{R})^3 \right) - 2 \left(1 - (\frac{a}{R})^3 \right) \right]}{\left(1 + \frac{a}{R} \left(\frac{1}{Bi} - 1 \right) \right) \left[1 + 2 \left(\frac{a}{R} \right)^3 + \nu - 4 \nu \left(\frac{a}{R} \right)^3 + \frac{2E}{3K} \left(1 - \left(\frac{a}{R} \right)^3 \right) \right]} \quad (3.9)$$

For the initially solid drop with fixed surface temperature the temperature distribution is substituted into (3.1) and (3.2) and the integration is given as:

$$\int_0^R \bar{T} r^2 dr = \frac{2K^2}{\pi^2} (T_{IN} - T_I) \left(\frac{e^{-\pi^2}}{4} + \frac{e^{-4\pi^2}}{4} + \frac{e^{-9\pi^2}}{4} \right) \quad (3.10)$$

$$\int_0^R \bar{T} r^2 dr = \frac{2K^2}{\pi^2} (T_{IN} - T_I) \left[e^{-\pi^2} \left(\frac{R}{\pi} \sin \frac{\pi r}{R} - r \cos \frac{\pi r}{R} \right) \right. \\ \left. - \frac{1}{4} e^{-4\pi^2} \left(\frac{R}{2\pi} \sin \frac{2\pi r}{R} - r \cos \frac{2\pi r}{R} \right) \dots \right] \quad (3.11)$$

For all four cases the stress distribution resembles a somewhat parabolic shape with a tensile stress at the surface of the solid and compressive on the interior. Specific examples of the stress distribution for both solid and liquid particles are given in Fig. 3.1 and 3.2 to illustrate the general stress behavior.

For the case of the liquid particles there is an increase in the material's density upon solidification. Thus a void will form within the interior of the liquid core. The tendency is then for the pressure stress to go to zero when this void is formed. In addition, due to the thermal stresses and the differential in temperature from its initially liquid state, the solid shell attempts to contract causing the pressure to increase. There are these two competing processes occurring during solidification. At some point in the process the void formation will contribute a larger volume of void than the decrease in volume associated with the contraction of the solid shell upon the compressible liquid core. At this point and beyond the internal pressurization will vanish and only thermal stresses will be present. The method of determining this delay

time when the volume of void created equals the volume of contraction is accomplished by examining the two processes separately. For the determination of void generation by density change a simplification is made to neglect buoyancy effects and assume the void formation occurs without inhibiting the formation of the solid shell. This is considered adequate for the present study.

If a mass balance is set up for the initially liquid drop (assuming as a first estimate R is fixed) the mass is

$$m = \rho_l V_0 = \rho_l \left(\frac{4}{3} \pi R^3 \right) \quad (3.12)$$

Later as solid shell is forming on the exterior the sum of the masses is given as

$$m = m_l + m_s \quad (3.13)$$

mass of solid is

$$m_s = \rho_s V_s = \rho_s \frac{4}{3} \pi (R^3 - a^3) \quad (3.14)$$

and mass of liquid is

$$m_l = \rho_l V_l = \rho_l \frac{4}{3} \pi (a^3 - R_{\text{void}}^3) \quad (3.15)$$

Now a void fraction is defined as

$$VF = \frac{V_{void}}{V_c} = \frac{V_c - (V_s + V_p)}{V_c} \quad (3.16)$$

Substituting in this equation, equations (3.12), (3.13) and (3.14) the final expression is found as

$$VF = \left(1 - \left(\frac{a}{R}\right)^3\right) \left(\frac{\rho_s}{\rho_l} - 1\right) \quad (3.17)$$

This then is the estimate of the void fraction increase due to the change in density of the solid.

To find the decrease in volume of the liquid due to the contraction of the internal radius (a) of the solid shell caused by thermal stresses and temperature Kent [14] uses the expression

$$\Delta r_{\theta} \Big|_{r=a} = \frac{a}{E} \left(\sigma_{\theta\theta} - \nu (\sigma_{rr} + \sigma_{\phi\phi}) \right) + \alpha a \bar{T}$$

Now again using the concept of void fraction the expression is given as

$$VF = \frac{4\pi a^2 \Delta r \Big|_{r=a}}{\frac{4}{3} \pi R^3} \quad (3.18)$$

$$VF = \frac{3 a^3 \Delta r \Big|_{r=a}}{R^3} \quad (3.19)$$

Note that in this second part of the analysis the external radius itself can change and contract inward according to (3.18) with "a" replaced by R. Thus an iterative solution of these two equations (3.17) and (3.19) can be done until the sum of the void fractions is zero. At this point and for solid shell thickness (R-a) greater than this, the internal pressurization is zero and a void has started to form. This analysis is shown in Fig. 3.3 for both the R fixed case and R varying. The results are not significantly different as is shown in the figure. The net result of the analysis indicates that for short times ($R=.005$ cm, $t=.000025$ sec) the stress within the solid shell will be due to both pressure and temperature. After the void formation due to the solid density increase has exceeded the shell thermal contraction, only thermal stresses will be acting on the spherical shell.

3.3 Fracture Mechanics and Stress Intensity Factors

The stresses developed by the temperature distribution within the solid are intensified when the solid shell has surface cracks or flaws within it. It is reasonable to assume that such flaws or cracks could exist on the solid spherical surface caused by voids due to fission gas release or pores in the microstructure. The fracture mechanics approach first utilized by Knapp [7] to explain this crack propagation, is employed in this report to predict the minimum radius of a fuel particle which will not fragment.

3.3.1 Brief Review of Fracture Mechanics

A very extensive review of fracture mechanics is given by Tetelman [17] and a brief summary of it is included here.

The basic view of fracture mechanics is that crack growth in a solid material under stress occurs when certain critical conditions are reached at the crack tip. Comparison of the conditions in the problem of interest are made with the critical conditions to determine if a crack will propagate. There are two types of material behavior in this determination; brittle and ductile.

The critical parameter which is used in the modeling of a brittle material is the fracture toughness (K_{IC}). For a given brittle material, all the combinations of loading and geometric types of cracks or flaws at the point of fracture will result in the same value of K_{IC} . Thus it is the critical constant for a brittle material to predict when a load-crack configuration will cause failure. The critical stress intensity factor as K_{IC} is sometimes called is a function of temperature and is a material property. For a particular loading and crack configuration the stress intensity factor (K_I) is determined. It is then compared to the fracture toughness of the material to determine if the material would survive such a loading without fracture. Stress intensity factors (K_I) have been determined for a number of simple geometries. The state of the art is summarized very well in a handbook by Tada [16].

To describe the conditions within the ductile region of a material, other methods of analysis have been developed. One which has been extensively used as an approximation to determine the zone

radius of the plastic deformation around the crack tip is given by Tetelman [17] as

$$r_y = c \left(\frac{K}{\sigma_y} \right)^2 \quad (3.20)$$

$c = \frac{1}{2\pi}$ plane stress

$\frac{1}{6\pi}$ plane stress

σ_y = yield stress

K = local stress intensity factor

r_y = plastic zone size

This parameter is not a measure of when a critical condition in the material is reached within the zone, but rather yields the size of the region affected by plastic deformation. It is strictly applicable only in the transition region between brittle and ductile material behavior. There are analytic tools being developed such as the energy line integral [7] for predicting ductile fracture, but their application to general problems is not widespread. Thus in trying to model the behavior of the material extended use is made of the brittle stress intensity factor. Knowing the material behavior of the fuel, a region of applicability for the stress intensity factor can be determined.

3.3.2 Limitations Due to Brittle Ductile Transition

Physically non-irradiated uranium dioxide undergoes a brittle-ductile transition between 1000 °C and 1400 °C. As Fig. 3.4 illustrates the fracture stress of pure non-irradiated UO_2 decreases at this transition with the stress given as [19]

$$\sigma_f = 15,000 + 3.7 T(^{\circ}\text{K}) \quad (3.21)$$

The implication of this behavior is that the use of the stress intensity factor K_I as a prediction of crack propagation will have limited applicability. It will be dictated by the portion of the solid which is in the brittle zone of behavior and extended into the brittle-ductile transition region only to a limited degree. Physically this means that if a crack or flaw exists on the surface of the solid and if the stress intensity factor (K_I) exceeds the fracture toughness (K_{IC}), the crack will propagate through the brittle material. But it will probably be blunted and stop when [7] it enters the brittle-ductile transition region, unless $K_I \gg K_{IC}$ as shown by Knapp [7]. At the crack tip the stresses cause some plastic deformation.

Extending this physical picture to the two types of particles under investigation (solid and liquid) some qualitative conclusions can be drawn. For the initially liquid droplet there are two limiting

physical boundaries which limit the growth of a surface crack or flaw if K_{IC} is exceeded by the stress intensity factor (K_I). The first is the brittle-ductile temperature transition zone which is located within the solid shell. The second and ultimate bound on crack propagation rate is the movement of the solid-liquid interface. It should be noted that both bounds on the propagation rate are due to the thermally controlled solidification process.

For the initially solid droplet a different condition exists where there is no interface movement and the temperature field within the solid decreases with time. Here the brittle-ductile transition boundary is the ultimate bound on the propagation rate. Again in this case the crack movement will probably be blunted within the ductile transition region of the particle. Thus the use of the brittle stress intensity factor as a prediction for fracture has strict validity only within the brittle region and will be extended partially into the brittle-ductile region.

The analysis used in this study is similar to that used by Knapp [7] and is based on a quasi-static evaluation of the stress intensity factor (K_I) at different time steps for a given crack size and a comparison with the fracture toughness K_{IC} . If the value of K_I exceeds K_{IC} , the crack within the solid particle will grow. The determination of the fracture toughness for the fuel material UO_2 is given by Knapp [7] as a function of temperature. Because of the variation of the temperature between bounds of 500

to 2800 °C the fracture toughness can vary from 2 to 3 (10^3) psi $\sqrt{\text{in}}$. In this problem these same temperatures are characteristic of the differential within the solid. Thus a mean K_{IC} of 2.5 (10^3) psi $\sqrt{\text{in}}$ is assumed with the understanding that an error band of about 50% exists around this mean value.

3.3.3 Stress Intensity Calculation

As was mentioned earlier, analytic expressions for the stress intensity factor (K_I) are available only for simple geometries [16]. In fact for the spherical geometry no solutions to the stress equation with a crack or flaw exist. The reason for this is that with a crack included on the surface of the sphere (whether solid shell or completely solid) the stress field is not rotationally symmetric and a three dimensional solution is required. As a first approximation to the spherical solution Blanel [18] suggested for thermally induced stresses with a crack present the form for K_I as

$$K_I = \frac{2.24\sqrt{C}}{\sqrt{\pi}} \int_0^C \frac{\sigma_t(r) d(R-r)}{\sqrt{C^2 - (R-r)^2}} \quad (3.22)$$

In reality this solution was derived for calculating the stress intensity factor for a plate with one face subject to sudden cooling and with a flaw at the cooled surface. This was obtained by superposition of the solution of the finite crack free plate with the solution of a cracked infinite plate [16]. The approximation made

to extend this to a spherical geometry is that for a solidifying liquid drop with thin solid shells, the thickness is small in comparison to the radius. Thus the solid shell surface can be approximated by a flat plate geometry. An error accompanying this approximation enters because the sphere is connected in the tangential directions so there is a constraint preventing the redistribution of stress at the crack tip. Therefore another bending moment occurs in the sphere that is nonexistent in the plate. As the curvature of the sphere becomes greater (R decreases) or the shell in the liquid drop becomes deeper, the plate approximation of K_I underestimates the real value. Some methods have been proposed to incorporate this error but these are limited to uniform stress fields which is not applicable here. The magnitude of the error is hard to determine because the real solution is not known [20]. As a rough estimate for the liquid case, only shell thicknesses of less than 20% of the initial drop radius are considered. For solids the K_I are known to be underestimated.

The second approximation associated with this solution is that it does not correct for the redistribution of the stress field for deep cracks. The solution is based on shallow cracks because they do not effect the stress field and the finite width plate behaves as if it were infinite. But if the initial crack is deep or if it grows and K_I is recomputed for a deep crack the actual stresses will be redistributed into the smaller area remaining and K_I is again underestimated. Blane [18] makes note of this and maintains that

although K_I will increase to a larger value than equation (4.22) predicts, the general form of the K_I variance with crack depth is valid. The magnitude of this error cannot be quantitatively determined. Therefore for this analysis the variance of K_I with crack depth will be assumed valid up to its maximum value (when $(C/R-a) \leq 0.25$) for each quasi-static calculation. This will be demonstrated within the following section. Therefore using the fracture mechanics approach to the problem introduces three major assumptions summarized below which will be viewed in light of the results of the analysis.

- a) Extension of brittle stress intensity calculation partially into the brittle-ductile transition zone.
- b) Usage of a stress intensity formula for plate geometries for spherical shells.
- c) No correction for stress redistribution due to crack depth.

4.0 RESULTS OF ANALYSIS

4.1 Progressive Crack Growth Evaluation

The cooling of the solid droplet or the solidification of the liquid droplet is a transient situation. The temperature distribution within the solid for both cases is time and position dependent, and the radius of the solid-liquid interface for the liquid particle decreases with time. Consequently the stresses developed within the solid and the accompanying stress intensity factor K_I are time dependent. The analysis which is used in this study is based on a quasi-static evaluation of K_I . At fixed times the temperature and stress fields are computed. Subsequently an analytical evaluation of K_I is made with the crack depth being varied parametrically at each fixed time step. This method gives the stress intensity factor for each time step for a variety of crack depths. Because of the limitation of the K_I expression of equation (3.22), the validity of this evaluation is suspect for crack depths greater than 20 to 25% of the solid thickness. This is illustrated in the following section.

The whole analysis was written into a computer program and used in this form for the K_I evaluation. The code is given in Appendix B, along with sample output for all four cases. To illustrate the logic of the code as written a flow chart of the major steps is given in Fig. 4.1. In the work done by Knapp [7], the size of liquid droplet investigated was for .36 cm. The results indicated that for all thicknesses of the spherical shell and for crack depths up to 80%

of the shell thickness the K_I values always exceeded (at least by a factor of 10) the fracture toughness K_{IC} .

The objective in this study is to determine the minimum size of droplet which will not fragment due to the sudden immersion in cold sodium coolant. The independent variables are the initial temperature of the sodium (T_{COOL}), the fixed interface temperature (T_I) of the particle or the heat transfer coefficient (h), theoretical temperature of the solid particle (T_{IN}), and the initial radius of the particle (R). The temperature of the sodium used in experimental investigations of fuel-coolant interactions has been in the range of 200 °C to 800 °C [2][4]. This range represents the upper and lower bounds of possible sodium temperatures under accident conditions for the Fast Flux Test Facility (FFTF). In this work the temperature is therefore varied throughout this range. The melting temperature of UO_2 is taken as 2800 °C for the liquid case and the initial temperature of the solid is parametrically varied from 2800 °C down to 1300 °C. The variation of the heat transfer coefficient is from .1 cal/scm² °C to 40 cal/scm² °C. These two values represent the bounds on a fission gas blanket and sodium nucleate boiling coefficients [7]. Physically the heat transfer coefficient's increase after about 20 cal/scm² °C has very little effect on the heat transfer process of the temperature distribution in solid fuel, because the thermal conductivity of the fuel controls the rate of heat transfer. The initial radius of the fuel droplet is the final independent variable. When the type of drop

(solid or molten) is specified along with its initial temperature, sodium temperature and surface boundary condition, the initial radius of the drop can be varied to find where the K_I values become equal to or fall below K_{IC} . This indicates that the particle has the capacity to survive the sudden cooling. In examining the results the initially solid or liquid particles will be discussed separately.

4.2 Results of Initially Liquid Particle

In the work done by Knapp [7] it was shown for initially large radius particles ($R=.36$ cm) that the stress intensity factors were at least a factor of ten greater than the fracture toughness for all initial thicknesses of the solidifying shell and for most depths of the crack. Because of this it was concluded that the crack would propagate through the shell and could cause fragmentation. By examination of the analytic expression for K_I it can be seen that as the initial radius of the drop decreases the stress intensity factor also decreases. The result indicates that K_I values always exceed the K_{IC} by a large margin until the initial radius is reduced to .01 cm, as Fig. 4.2 illustrates. For the severe conditions within the reactor of the lowest sodium temperature (200 °C) and perfect wetting of the solid and liquid ($T_I = 945$ °C) interface, the K_I values are of the same order of magnitude as the fracture toughness. The graph indicates by the solid lines the region of validity of the K_I evaluation and by the short dashed lines where it underestimates the actual values. Superimposed upon this graph

are the regions of brittle, brittle-ductile, and ductile behavior for the UO_2 solid shell. Because the abscissa of the graph is dimensionless distance, the temperature boundaries appear as vertical lines although in reality they move inward toward the center with time. As the graph indicates in the brittle region of UO_2 the K_I values of the fuel exceed the fracture toughness by a small amount. This implies that the crack will grow. But as it does, it enters the brittle region of UO_2 . Here the crack growth will probably be arrested and plastic deformation will occur. This scenario is feasible because the K_I values are not significantly greater in the brittle region than K_{IC} (given the associated error band of 50% for the fracture toughness). The crack grows but can be easily stopped and the stresses at the tip blunted by plastic deformation. This is in contrast to a larger drop where K_I is much greater, thus the probability of propagation further into the ductile zone before being blunted and stopped is greater. As Knapp [7] concluded for .36 cm ($K_I > 10K_{IC}$), in all likelihood the crack could go through the whole shell since its kinetic energy is so great. So the conclusion here is that in the range of .01 cm initial drop radius the stress intensity factors are greater than K_{IC} but of the same order of magnitude. For a smaller radius of .005 cm as is illustrated in Fig. 4.3, the K_I values are slightly above K_{IC} in the brittle ductile region but are below K_{IC} in the brittle region near the surface of the shell. So it appears that the possibility

exists for a liquid particle of the size range .005 cm to survive a sudden cooling as in a fuel-coolant interaction. The first curve in Fig. 4.3 illustrates the case where the thermal and pressure tangential stresses are both acting on the shell. After a short time as the past analysis has shown in Section 3.2, the void in the liquid core forms and the pressurization vanishes leaving only thermal stresses as is shown by curves 2 and 3 for K_I . This minimum size range of about 50 μ m in size has been shown experimentally where the same conditions as assumed here were used [4]. This type of analysis then illustrates an upper bound on the size of a survivable particle in a FCI of about 50 μ m radius with the given temperature conditions.

The next step is to vary the other independent parameters to determine their effect on the K_I values within this size range of particles. If the fixed interface temperature condition is kept but the sodium coolant temperature is raised to values in the operating range of the FFTF and above, results as shown in Fig. 4.4 are obtained. The graph illustrates that for fixed T_I , the variance of the sodium coolant temperature has the effect of reducing the stress intensity factors by about 25%-35%. A shell thickness (a/R) of .87 is used to illustrate this variance of the maximum value of K_I for various values of T_{COOL} . This behavior is representative of all shell thicknesses during the solidification process. This variance does not affect to a large extent the results of the minimum radius for no fragmentation. The reason is that the error band on

K_{IC} is around $\pm 25\%$ thus the 25% variance in stress intensity factor will not change the overall conclusion on this upper bound of 50 μm .

The next parameter which is varied is the surface boundary condition from a perfect wetting situation to a finite heat transfer coefficient (h). This variance is based upon the upper limit of 40 $\text{cal}/\text{scm}^2 \text{ } ^\circ\text{C}$ for nucleate boiling of sodium vapor and a lower limit of .1 $\text{cal}/\text{scm}^2 \text{ } ^\circ\text{C}$ based on fission gas blanket [7]. Unlike the variance of T_{COOL} , the sensitivity of the stress intensity factor to the heat transfer is quite significant for low values of h as illustrated in Fig. 4.5. Again a shell thickness (a/R) of .9 is employed to illustrate the general behavior of K_I values with h variance. For values of h greater than 10 $\text{cal}/\text{scm}^2 \text{ } ^\circ\text{C}$, the variance in K_I is minor. This is due to the fact that the thermal conductivity of the solid fuel controls the heat transfer process (Biot number is larger than 10), thus limiting the effect of large h . For lower heat transfer coefficients around 2 $\text{cal}/\text{scm}^2 \text{ } ^\circ\text{C}$ (similar to sodium film boiling) the K_I values are reduced significantly by a factor of five. The point to remember is that an approximate solution to the energy equation is used to determine the temperature distribution within the solid shell. So as Fig. 2.4 generally illustrates the temperature difference (between $R(r,t) - T_m$) given by the London and Seban method is greater than reality. Thus the stresses and K_I values are over-estimated for longer times. To see how this reduction in K_I affects the minimum size of fuel particle which can survive fragmentation, consider the graph in Fig. 4.6. This graph gives the K_I values at

their maximum values approximately 20% into the shell thickness and halfway into the brittle ductile transition zone. On the left of the graph are the asymptotic values of K_I for fixed T_I condition. As the heat transfer coefficient decreases the minimum size of particle that can survive fragmentation increases. By this first order analysis it appears that a particle of 100 μm could survive fragmentation when the heat transfer coefficient is in the range of 1 to 10 $\text{cal}/\text{scm}^2 \text{ } ^\circ\text{C}$, and a larger particle of 500 μm in radius could survive if a fission gas blanket were around the particle initially ($h \sim .1-.15 \text{ cal}/\text{scm} \text{ } ^\circ\text{C}$). The brittle-ductile behavior of the fuel must be considered in light of these conclusions. In actuality the material will plastically deform to blunt crack growth making the size of the particle which can survive fragmentation larger. For a variance in the sodium coolant temperature the results are similar to the fixed temperature case as shown in Fig. 4.7. The effect of raising T_{COOL} results in a 25% reduction in the K_I values. This does not have a significant impact upon the survivable size of a fuel particle. Thus the surface boundary conditions has the largest impact upon the minimum fuel particle size.

4.3 Results for the Initially Solid Particle

The same analysis has been carried out for an initially solid particle with fixed interface temperature. The major differences in the behavior of the K_I values are exhibited by Fig. 4.8. For the case of the solidifying liquid the stress intensity factors increase with time because the solid shell becomes thicker and

because the stresses are larger. Eventually near the end of solidification, stresses decrease as do the K_I values. In contrast, for a solid, the stress intensity factors initially are large, and decrease rapidly with time as Fig. 4.8 illustrates. The reason for their initial magnitude is that the temperature distribution is sharply skewed with temperatures near the initial value within a large portion of the solid and temperature near the coolant temperature only at the surface of the solid. This generates large tensile stresses at the surface and causes K_I to be large. As time progresses the sphere's temperature decreases to such an extent that the gradient of the temperature across the radius is lowered and the stresses decrease quickly.

The final point to remember is that the brittle-ductile transition zone moves with time from the surface of the sphere toward the center. Initially almost the entire sphere is above 1000 °C. As the graph indicates the only brittle region is near the surface and cracks can grow there, because K_I is larger than K_{IC} . But because the crack enters the brittle-ductile transition region its progress is not likely. Only if the brittle-ductile zone occupies a small percentage of the volume of the particle and K_I is larger than K_{IC} could a crack expect to propagate deep within the particle and fragmentation occur. This combination of conditions is not fulfilled for the 50 μm size because at very short times K_I falls below K_{IC} , before the transition zone has moved more than 10% into the particle.

The conclusion then is that a solid particle can be larger in radius than 50 μm and still not fragment. The reason for this physically is due to the fact that in the liquid case the molten core is an energy supply which keeps the interior temperature high and the gradient large. For the solid the interior temperature decreases with time, therefore the gradient decreases as do the stresses. Figure 4.9 illustrates that for a particle of 100 μm radius the K_I values are substantially higher than K_{IC} even after a large percentage of the volume is in the brittle region. Thus the crack would propagate and fragmentation is likely to occur. This result then illustrates that minimum size of solid particles is greater than 50 μm , but is smaller than a particle of 100 μm radius which could fragment.

The final independent variable which is varied is the temperature difference of the initial temperature of the solid and the sodium coolant. The difference of the two temperatures is what governs the magnitude of the stresses that are induced in the solid. The initial temperature of the particle is varied because physically the initial temperature depends upon where the solid particle originated. If it fragmented from the surface of the solidified shell of a larger drop, it would be at a temperature in the range of 1000-1300 $^{\circ}\text{C}$. However if it broke off with the thickness of the whole thin shell of a liquid drop or from an interior portion of the shell, the temperature would be closer to the melting temperature. The reality of a skewed initial temperature distribution cannot be handled easily mathematically. Therefore as a conservative estimate, a value of

$T_{IN} - T_m$ is used. The former case of surface fragmentation has been shown to be more feasible for an initially liquid droplet, because cracks will probably be blunted as they progress toward the interior of the solidifying shell. As Fig. 4.10 illustrates the variance of the temperature differential for solids has a much more dramatic effect than for liquid droplets. Over the differential temperature range of 50 to 2600 °C the variance in K_I values is approximately 300-400%. The implication of this is that many of the larger particles observed in experimental results [4] which survive the fuel coolant interaction could originate from this mechanism. The solid particle is fragmented from a larger solidifying liquid droplet. Because it comes from the outer brittle surface of the solid shell it is at a relatively low temperature (1000-1300 °C) and will not fragment any further.

Now consider the solid particle with a fixed heat transfer coefficient as illustrated in Fig. 4.11. Similar behavior to the liquid case is shown when the heat transfer coefficient (h) is lowered. The maximum K_I values for a given time step decrease as h decreases, because the temperature distribution within the drop is not as skewed, thus the tangential thermal stresses decrease. Another behavior to notice is that as the h decreases the quantitative decrease of K_I with each time step lessens. This occurs because the temperature distribution requires a longer time to be redistributed to a uniform level which results in stress levels remaining higher over longer periods of time. Additionally the

brittle ductile transition zone of the material remains closer to the surface of the solid over longer periods of time. The net effect is then to allow crack growth primarily in the brittle region which is still not a large portion of the body. As Fig. 4.12 illustrates the possibility of larger solid particles surviving a fuel coolant interaction for the worst differential increases as heat transfer coefficient decreases. The conclusion though is not changed significantly. For high heat transfer coefficients (10-30 cal/scm² °C) the minimum particle which can withstand the transient thermal stresses is around the 50 μm size range.

The final variance to examine is the temperature differential ($T_{IN} - T_{COOL}$) for a fixed heat transfer coefficient in Fig. 4.13. Similar to Fig. 4.10 the general effect of a decrease in $T_{IN} - T_{COOL}$ is dramatic. The same argument should hold for the likelihood of decreased temperature differentials and increased non-fragmented solid particle sizes.

5.0 CONCLUSIONS

This analysis has illustrated two primary things. First a bound on the minimum size of a fuel particle which could survive on immersion into sodium coolant without fragmentation has been found. The size range determined by this analysis of about 50 μm radius is within the recently observed experimental minimum particle size. Secondly when the material behavior of UO_2 with temperature is considered along with this thermal stress fracture model a mechanism of fragmentation can be visualized. If a larger particle of molten fuel is immersed into the sodium coolant it will start to solidify. Within the outer solid surface of the spherical shell the material behavior will be brittle. Thus for larger radius $K_I > K_{IC}$, and any surface flaws will be propagated through the solid. If $K_I \gg K_{IC}$ then the likelihood of crack fracture into the ductile zone of UO_2 and complete rupture of the solid shell is increased. This will result in large solid particles and liquid particles being released from the shell. The solid particles are given off with very skewed temperature distributions. Because the initial temperature is close to T_m , these particles will fragment subsequently. This will continue until the temperature within the solid decreases below a value that $K_I < K_{IC}$ or the fragments are of a size such that $K_I < K_{IC}$. For these conditions fragmentation will cease. If $K_I > K_{IC}$ by a small degree, the fragmentation will occur only in the outer brittle region of the shell yielding smaller solid particles which will probably not fragment to such a large extent because either

their initial temperatures are low and $K_I < K_{IC}$ or the ductile region will blunt crack growth. Additionally there is the possibility of a lower finite heat transfer coefficient which will allow larger particles to survive without fragmentation. Thus this scenario illustrates the possibility that the thermal stress fracture mechanism can explain the fragmentation process. A final observation to be drawn from this analysis stems from this minimum possible fragmentation size of 50 microns radius. This size particle is at least an order of magnitude too large to become airborne and inhaled in the human lung as a possible toxic agent to human health.[2]

This analysis is based upon an approximate fracture model of the phenomena. The assumptions employed to use this model dictate that it can only be considered as a first order approximation to predict the phenomenon. Future work should be directed into the fracture mechanics area of the problem. The expected results of such an investigation do not appear to be easily obtained.

APPENDIX A
MATERIAL PROPERTIES

UO₂

$$k_s = .005 \text{ cal/sec cm } ^\circ\text{C}$$

$$\rho_s = 11 \text{ gm/cm}^3$$

$$c_p = .11 \text{ cal/gm } ^\circ\text{C}$$

$$K = 4 \times 10^6 \text{ psi}$$

$$E = 26.5 \times 10^6 \left(1. - \frac{0.6T(C)}{2700}\right) \text{ psi}$$

$$\alpha = \left(4.2 + \frac{2.8}{2000} T(F)\right) \times 10^{-6} \text{ in/in } ^\circ\text{F}$$

$$T_m = 2800 \text{ } ^\circ\text{C}$$

$$\nu = .5$$

$$\rho_\ell = 8.74 \text{ gm/cm}^3$$

$$L = 67 \text{ cal/gm}$$

Na

$$k_c = .184 \text{ cal/sec cm } ^\circ\text{C}$$

$$\rho = .896 \text{ gm/cm}^3$$

$$c_p = 0.30 \text{ cal/gm } ^\circ\text{C}$$

$$T_c = 200 - 450 \text{ } ^\circ\text{C}$$

APPENDIX B

SOLUTION TECHNIQUE

The purpose of this appendix is to summarize the basic components of the computer aided solution to the thermal stress fracture model. This will allow future workers a chance to use, understanding and hopefully extend this model.

The program can be thought as consisting of five parts. The first four parts consist of the main program where each part corresponds to the type of particle being analyzed (solid or liquid, fixed T_I or h). Within each of these sections there are two DO loops. The outer one increments the time step. This is done for the liquid by fixing the solid-liquid interface position (a) and finding the time to solidify to that point. For the solid the time (t) is incremented directly. The inner loop divides the solid (whether the shell for the liquid case or the particle for the solid) into discrete sections and increments the radius to each of these. At each fixed radius the temperature and stress is calculated (either analytically or by numerical integration) and stored in an array, with

S6(J) - Tangential Pressure Stress

S7(J) - Radial Pressure Stress

S8(J) - Tangential Thermal Stress

S9(J) - Radial Thermal Stress

Once the whole solid is traversed the fifth component is called by a subroutine. This is the section SUBROUTINE CONFAC which calculates the stress intensity factor. The stress in eqn. (4.22) is approxi-

mated by either a linear model ($\sigma_t = A_1(R-r) + B_1$) or quadratic model ($\sigma_t = A_1(R-r)^2 + B_1(R-r) + C_1$). The choice depends upon the deviation of the stresses from a linear profile. For all cases in this study the stresses were parabolic thus the quadratic expression is used.

The depth of the crack at the surface is varied over the thickness of the solid thus giving the variance in K_I .

The remaining subprograms in the code are associated with numerical integration of the stress equation for the liquid (fixed T_I) and solid (fixed $\bar{h}$) cases. The details of the programs should be understandable.

The input determines the type of drop analyzed, its radius and all the other physical parameters needed for analysis. In the example output the variable input parameters are listed. The program is easily modified to handle more than one case at a time by the installation of an outer DO LOOP so that more data can be read into the program and executed.

C
 C INPUT VARIABLES
 C
 C
 C ALPHA=THERMAL CONTRACTION COEFFICIENT
 C ANU=POISSON'S RATIO
 C APPRL DEVIATION OF STRESS CALCULATED TO AVERAGE
 C BDC TYPE OF BOUNDARY CONDITION 1- FIXED T1 2-FIXED H
 C BIOT DIMENSIONLESS PARAMETER $H \cdot R / K$
 C BULK=BULK MODULUS OF THE FUEL
 C CDEP INITIAL CRACK DEPTH
 C CFIN PROPORTION OF TOTAL DEPTH THAT CRACK PARAMETRICALLY PROGRESSES
 C DROP TYPE OF DROP 1-SOLID 2-LIQUID
 C E=YOUNG'S MODULUS
 C HTC INTERFACE HEAT TRANSFER COEFFICIENT
 C L=INTEGRATION SUBDIVISIONS (SIMPSON'S RULE)
 C LM=INTEGRATION SUBDIVISIONS (SIMPSON'S RULE)
 C M=NUMBER OF RADIAL POSITIONS ACROSS THE SHELL FOR STRESS CALCS.
 C NM=NUMBER OF SURFACE TEMPERATURE VALUES USED (INTERFACE)
 C NN=NUMBER OF SOLIDIFICATION FRONT POSITIONS
 C R=OUTSIDE DROP RADIUS
 C RHOSF DENSITY OF SOLID FUEL
 C RHOLF DENSITY OF LIQUID FUEL (MEAN TEMP)
 C SL=LATENT HEAT OF SOLIDIFICATION
 C SPHT=SPECIFIC HEAT OF SOLIDIFYING MATERIAL
 C TCOOL INITIAL TEMPERATURE OF COOLANT
 C TDEL TIME INCREMENT FOR SOLID SPHERE
 C THCONF FUEL THERMAL CONDUCTIVITY
 C THCONC COOLANT THERMAL CONDUCTIVITY
 C THI=HIGHEST INTERFACE TEMPERATURE DESIRED
 C TI=INTERFACE TEMPERATURE
 C TIN INITIAL TEMPERATURE OF SOLID FUEL SPHERE
 C TLOW=LOWEST INTERFACE TEMPERATURE DESIRED
 C TM=MELTING POINT OF THE FUEL
 C TS=THERMAL DIFFUSIVITY OF THE SOLIDIFYING MATERIAL
 C ZZ=FINAL POSITION OF SOLIDIFICATION FRONT
 C

```

ISN 0002      DIMENSION A(25),RAD(100),S6(25),S7(25),S8(25),S9(25),SIGK(100)
ISN 0003      COMMON R,SPHT,TM,TI,SL,TS,OADT,B,TBAR
ISN 0004      COMMON FO,T,RHOSF,AZ,THCONF,AY1,AY2,AY3,AY4,AY5,TIN
ISN 0005      COMMON APPRL
ISN 0006      READ(5,600) DROP , BDC, APPRL
ISN 0007      600 FORMAT(2F5.2,F10.2)
ISN 0008      READ(5,200)ILM,TS,SL,BULK,TN,ANU
ISN 0009      200 FORMAT(I4,F7.5,F5.0,F10.0,F5.0,F5.4)
ISN 0010      READ(5,300)MM,THI,TLOW,ALPHA,E
ISN 0011      300 FORMAT(I4,2F5.0,F10.7,F10.0)
ISN 0012      READ(5,800) RHOSF, RHOLF, RH,TI
ISN 0013      800 FORMAT(4F10.4)
ISN 0014      READ(5,900) THCONF,THCONC,TCOOL,TIN,TDEL,TFIN
ISN 0015      900 FORMAT(6F10.4)
ISN 0016      READ(5,100)NN,M,L,R,ZZ,SPHT
ISN 0017      100 FORMAT(3I4,3F5.4)

```

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ISN 0018      READ(5,700) BIOT,CDEP,HTC
ISN 0019      700 FORMAT(3F10.4)
ISN 0020      WRITE(6,2001) R,ALPHA,E
ISN 0021      2001 FORMAT(' R',F7.5,' ALPHA',E12.4,' E',F15.4)
ISN 0022      WRITE(6,2002) BIOT,HTC,TCOOL,TIN
ISN 0023      2002 FORMAT(' BIOT',F8.4,' HTC',F8.4,' TCOOL',F8.2,' TIN',F8.2)
ISN 0024      IF(DROP-1.)60,61,62
ISN 0025      60 GO TO 98
ISN 0026      62 IF(BDC-1.)60,63,64
ISN 0027      63 TCHG=(THI-TLOW)/FLOAT(MM-1)
ISN 0028      EXTERNAL FUNCT,FCT2
ISN 0029      DO 50 II=1,MM
ISN 0030      T1=THI-TCHG*FLOAT(II-1)
ISN 0031      R1=0.0
ISN 0032      R2=B

```

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ISN 0070      DELR=RAD(1)*(S8(1)-ANU*(S8(1)+S9(1)))/E
ISN 0071      RVOID=R*((RHOSF/RHOLF - 1.)*(1.-B/R))**.33
ISN 0072      RVF=(RVOID/R)**3
ISN 0073      RTF=3.*(B**2.)*DELR/(R**3.)
ISN 0074      IF(RVF+RTF)68,68,67
ISN 0075      68 SIGK(J)= S6(J)+ S8(J)
ISN 0076      WRITE(6,8001) S6(J),S8(J)
ISN 0077      8001 FORMAT(' TAN PRESS ',3X,E12.6,' TAN THERMAL ',3X,E12.6)
ISN 0078      GO TO 69
ISN 0079      67 SIGK(J)=S8(J)
ISN 0080      WRITE(6,8002) S8(J)
ISN 0081      8002 FORMAT(' TAN THERMAL ',3X,E12.6)
ISN 0082      69 CONTINUE
ISN 0083      2 CONTINUE
ISN 0084      CALL CONFAC(SIGK,R,B,M,CDEP)
ISN 0085      1 CONTINUE
ISN 0086      50 CONTINUE
ISN 0087      GO TO 99
ISN 0088      64 ACHG=0.0
ISN 0089      DRAD=0.0
ISN 0090      ACHG=(R-ZZ)/FLOAT(NN-1)
ISN 0091      DO 5 I=2,NN
ISN 0092      A(I)=R-ACHG*FLOAT(I-1)
ISN 0093      TC1=(1./BIOT-1.)*(1.-(A(I)/R)**3.)/3.
ISN 0094      TC2=(1.-(A(I)/R)**2.)/2.
ISN 0095      TC3=(SL*(R**2.))/(THCONF*TM)
ISN 0096      B=A(I)
ISN 0097      TIME=TC3*(TC1+TC2)
ISN 0098      WRITE(6,5000) B,TIME
ISN 0099      5000 FORMAT(' INTERFACE POSITION=',F9.8,6X,' TIME=',F12.6)
ISN 0100      DRAD=(R-A(I))/FLOAT(M-1)
ISN 0101      DO 6 J=1,M
ISN 0102      RAD(J)= B+DRAD*FLOAT(J-1)
ISN 0103      RI=RAD(J)
ISN 0104      SHEL=B/R
ISN 0105      TPS1=3.*(SHEL-SHEL**3.)
ISN 0106      TPS2=2.*(1.-SHEL**3.)
ISN 0107      TPS3=(1.+SHEL*(1./BIOT-1.))
ISN 0108      TPS4=(1.+2.*SHEL**3.+ANU-4.*ANU*(SHEL**3.))
ISN 0109      TPS5=(2./3.)*(E/BULK)*(1.-SHEL**3.)
ISN 0110      TPS6=E*(TN-TCOOL)*ALPHA
ISN 0111      PRE=(TPS6)*(TPS1+TPS2)/(TPS3*(TPS4+TPS5))
ISN 0112      S6(J)=(PRE*B**3.)*(2.*RI**3.+R**3.)/(2.*RI**3.*(B**3.-R**3.))
ISN 0113      ITS1=2.*ALPHA*E*(TN-TCOOL)/(1.-ANU)

```

```

ISN 0114      RRI=R1/R
ISN 0115      TTS2=(2.*RRI**3.+SHEL**3.)/(2.*(1.-SHEL**3.)*(RRI**3.))
ISN 0116      TTS3=.5*(SHEL-SHEL**3.)-(1.-SHEL**3.)/3.
ISN 0117      TTS4=1.+SHEL*(1./BIOT-1.)
ISN 0118      TTS5=.5*SHEL*(RRI**2.-SHEL**2.)/(2.*RRI**3.)
ISN 0119      TTS6=-1.*(RRI**3.-SHEL**3.)/(6.*RRI**3.)
ISN 0120      TTS7=.5*(SHEL/RRI-1.)
ISN 0121      S8(J)=TTS1*(TTS2-TTS3/TTS4+(TTS5+TTS6)/TTS4-TTS7/TTS4)
ISN 0122      DELR=RADI(1)*S8(1)*(1.-ANU)/E
ISN 0123      RVOID=R*((RHOSF/RHOLF - 1.)*(1.-B/R))**.33
ISN 0124      RVF=(RVOID/R)**3.
ISN 0125      RTF=3.*(B**2.)*DELX/(R**3.)
ISN 0126      IF(RVF+RTF)73,73,74
ISN 0127      73 SIGK(J)=S8(J)+S6(J)

ISN 0128      WRITE(6,8003) S6(J),S8(J)
ISN 0129      8003 FORMAT(' TAN PRESS ',3X,E12.6,' TAN THERMAL ',3X,E12.6)
ISN 0130      GO TO 75
ISN 0131      74 SIGK(J)=S8(J)
ISN 0132      WRITE(6,8004) S8(J)
ISN 0133      8004 FORMAT(' TAN THERMAL ',3X,E12.6)
ISN 0134      75 CONTINUE
ISN 0135      6 CONTINUE
ISN 0136      CALL CONFAC(SIGK,R,B,M,CDEP)
ISN 0137      5 CONTINUE
ISN 0138      GO TO 99
ISN 0139      61 IF(BDC-1.)60,66,65
ISN 0140      66 TRE=0.0
ISN 0141      PE=TS*(3.1416/R)**2.
ISN 0142      PREF=E*ALPHA/(1.-ANU)
ISN 0143      80 CONTINUE
ISN 0144      TRE=TRE+TDEL

```

```

ISN 0145      WRITE(6,6000) TRE
ISN 0146      6000 FORMAT(' TIME=',6X,F8.5)
ISN 0147      T=TRE
ISN 0148      DRAD=R/FLOAT(M)
ISN 0149      DO 7 J=1,M
ISN 0150      RAD(J)=DRAD*FLOAT(J)
ISN 0151      RI=RAD(J)
ISN 0152      SRS1=2.*(TIN-TI)/(3.1416**2.)
ISN 0153      AG=-1.*PE*T
ISN 0154      SRS2=EXP(AG)+EXP(4.*AG)+EXP(9.*AG)+EXP(16.*AG)
ISN 0155      SRS3=EXP(25.*AG)+EXP(36.*AG)
ISN 0156      AX=3.1416*RI/R
ISN 0157      SRS4=SRS1*(R**2.)/(RI**3.)
ISN 0158      SRS5=EXP(AG)*(R*SIN(AX)/3.1416-RI*COS(AX))
ISN 0159      SRS6=.25*EXP(4.*AG)*1.5*R*SIN(2.*AX)/3.1416-RI*COS(2.*AX)
ISN 0160      SRS7=EXP(9.*AG)*(R*SIN(3.*AX)/9.4248-RI*COS(3.*AX))/9.
ISN 0161      SRS8=EXP(16.*AG)*(R*SIN(4.*AX)/12.5664-RI*COS(4.*AX))/16.
ISN 0162      SRS9=EXP(25.*AG)*(R*SIN(5.*AX)/15.708-RI*COS(5.*AX))/25.
ISN 0163      SRS10=EXP(36.*AG)*(R*SIN(6.*AX)/18.8496-RI*COS(6.*AX))/36.
ISN 0164      SRS12=(2.*R/(3.1416*RI))*(TIN-TI)
ISN 0165      SRS13=EXP(AG)*SIN(AX)-EXP(4.*AG)*SIN(2.*AX)/2.
ISN 0166      SRS14=EXP(9.*AG)*SIN(3.*AX)/3.-EXP(16.*AG)*SIN(4.*AX)/4.
ISN 0167      SRS15=EXP(25.*AG)*SIN(5.*AX)/5.-EXP(36.*AG)*SIN(6.*AX)/6.
ISN 0168      SRSM=2.*SRS1*(SRS2+SRS3)+SRS4*(SRS5-SRS6+SRS7-SRS8+SRS9-SRS10)
ISN 0169      SRSE=-1.*SRS12*(SRS13+SRS14+SRS15)
ISN 0170      SIGK(J)=PEF*(SRSM+SRSE)
ISN 0171      WRITE(6,8005) SIGK(J)
ISN 0172      8005 FORMAT(' TAN THERMAL ',3X,E12.6)
ISN 0173      7 CONTINUE
ISN 0174      CALL CONFAC(SIGK,R,RH,M,CDEP)
ISN 0175      IF(TRE-TFIN)80,81,81
ISN 0176      81 GO TO 99
ISN 0177      65 TRE=0.0
ISN 0178      TRAD1=3.*HTC/(R*RHDSF*SPHT)
ISN 0179      TRAD2=R*HTC/(5.*THCONF)
ISN 0180      TRAD3=2.*R*HTC/THCONF
ISN 0181      90 CONTINUE
ISN 0182      TRE=TRE+TDEL
ISN 0183      WRITE(6,7000) TRE
ISN 0184      7000 FORMAT(' TIME=',6X,F8.5)
ISN 0185      T=TRE

```

```

ISN 0186      AZ=-1.*TS*T/(R**2.)
ISN 0187      AY1=4.49**2.
ISN 0188      AY2=7.725**2.
ISN 0189      AY3=10.9**2.
ISN 0190      AY4=14.07**2.
ISN 0191      AY5=17.22**2.
ISN 0192      SUM1=EXP(AZ*AY1)/AY1+EXP(AZ*AY2)/AY2+EXP(AZ*AY3)/AY3
ISN 0193      SUM2=EXP(AZ*AY4)/AY4+EXP(AZ*AY5)/AY5
ISN 0194      TRAD4=TCOOL*(TRAD1*T+TRAD2-TRAD3*(SUM2+SUM1))+TIN
ISN 0195      TRAD5=(TRAD4-TIN)/TCOOL
ISN 0196      TRAD=TRAD4/(TRAD5+1.)
ISN 0197      FO=HTC*(TCOOL-TRAD)
ISN 0198      R5=R
ISN 0199      R6=0.0
ISN 0200      LL=LM
ISN 0201      DRAD=R/FLOAT(M)
ISN 0202      DO 8 J=1,M
ISN 0203      RAD(J)=DRAD*FLOAT(J)
ISN 0204      R7=RAD(J)
ISN 0205      EXTERNAL FCT3
ISN 0206      AINT5=SINPS(R6,R5,L,FCT3)
ISN 0207      AINT6=SINPS(R6,R7,LL,FCT3)
ISN 0208      LL=LL+2
ISN 0209      PRE9=E*ALPHA/(1.-ANU)
ISN 0210      S9(J)=2.*PRE9*(AINT5/(R**3.)-AINT6/(R7**3.))
ISN 0211      TBAR1=FCT3(R7)/R7**2.
ISN 0212      S8(J)=PRE9*(2.*AINT5/(R**3.)+AINT6/(R7**3.)-TBAR1)
ISN 0213      WRITE(6,8006) S8(J)
ISN 0214      8006 FORMAT(' TAN THERMAL ',3X,E12.6)
ISN 0215      SIGK(J)=S8(J)
ISN 0216      8 CONTINUE
ISN 0217      CALL CONFAC(SIGK,R,RH,M,CDEP)
ISN 0218      IF(TRE-TFIN)90,91,91
ISN 0219      91 GO TO 99
ISN 0220      98 CONTINUE
ISN 0221      99 CONTINUE
ISN 0222      STOP
ISN 0223      END

```

```

ISN 0002      SUBROUTINE CONFAC(SIGK,R,B,M,CDEP)
ISN 0003      COMMON APPRL
ISN 0004      DIMENSION SIGK(100)
ISN 0005      SIGM=(SIGK(M)+SIGK(1))/2.
ISN 0006      K=(M-1)/2+1
ISN 0007      SIGMD=SIGK(K)
ISN 0008      CF=R-B
ISN 0009      WRITE(6,9005) CF
ISN 0010 9005  FORMAT('  CF  ',3X,F9.8)
ISN 0011      CIN=CF/10.0
ISN 0012      CDEPP=CDEP
ISN 0013      DEVT=ABS(SIGM-SIGMD)
ISN 0014      IF(DEVT-APPRL)70,71,71
ISN 0015 70    CONTINUE
ISN 0016      SCFK=0.0
ISN 0017      CDEPP=CDEPP+CIN
ISN 0018      COMP1=SIGK(M)*1.5708
ISN 0019      COMP2=CDEPP*(SIGK(M)-SIGK(1))/(R-B)
ISN 0020      SCFK=.79297*(COMP1-COMP2)*(CDEPP**.5) + SCFK
ISN 0021      WRITE(6,3000) CDEPP,SCFK
ISN 0022 3000  FORMAT(' CRACK DEPTH(CM)',F9.8,6X,'K-I FACTOR(L)(P/13/2)',E12.4)
ISN 0023      IF(CDEPP-CF) 70,76,76
ISN 0024 71    CONTINUE
ISN 0025      SCFK=0.0
ISN 0026      CDEPP=CDEPP+CIN
ISN 0027      COMPA=2.*(SIGK(M)+SIGK(1)-SIGMD)/(R-B)**2.1
ISN 0028      COMPB=(4.*SIGMD-3.*SIGK(M)-SIGK(1))/(R-B)
ISN 0029      COMPD=SIGK(M)
ISN 0030      SUBT=.7854*COMPA*(CDEPP**2.)+COMPB*CDEPP+COMPD*1.5708
ISN 0031      SCFK=.79297*SUBT*(CDEPP**.5)+SCFK
ISN 0032      WRITE(6,4000) CDEPP,SCFK
ISN 0033 4000  FORMAT(' CRACK DEPTH(CM)',F9.8,6X,'K-I FACTOR(Q)(P/13/2)',E12.4)
ISN 0034      IF(CDEPP-CF)71,76,76
ISN 0035 76    CONTINUE
ISN 0036      RETURN
ISN 0037      END

```


ISN 0002	FUNCTION FCT2(Y)
ISN 0003	COMMON R,SPHT,TM,TI,SL,TS,DADT,B,TBAR
ISN 0004	GRP1=(SL/1TS*SPHT1)*(R-Y)/(R*Y)*B**2.*DADT
ISN 0005	GRP2=B*DADT**2*SL/SPHT*((1./TS)**2.)*((R-Y)/(R-B))*(R/3.-Y/6.-B**
	12./(2.*Y)+B**3./(3.*R*Y))
ISN 0006	TBAR=TI-GRP1+GRP2-TM
ISN 0007	FCT2=TBAR*Y**2.
ISN 0008	RETURN
ISN 0009	END

ISN 0002	FUNCTION FUNCT(Y)
ISN 0003	COMMON R,SPHT,TM,TI,SL,TS
ISN 0004	DENOM=2.*TS*SPHT*(TM-TI)
ISN 0005	Z=1.0+((4.*R*SPHT)/(3.*Y*SL))*(TM-TI)
ISN 0006	DENUM=(SL*Y-(SL*Y**2.)/R)*(1.0+SQRT(Z))
ISN 0007	FUNCT=DENUM/DENOM*(-1.0)
ISN 0008	RETURN
ISN 0009	END

ISN 0002	FUNCTION SIMPS(D,E,N,F)
ISN 0003	TWOH=(E-D)/FLOAT(N)
ISN 0004	H=TWOH/2.
ISN 0005	SUMED=0.0
ISN 0006	SUMID=0.0
ISN 0007	DO 10 K=1,N
ISN 0008	X=D+FLOAT(K-1)*TWOH
ISN 0009	SUMED=SUMED+F(X)
ISN 0010	SUMID=SUMID+F(X+H)
ISN 0011	10 CONTINUE
ISN 0012	SIMPS=(2.0*SUMED+4.0*SUMID-F(D)+F(E))*H/3.
ISN 0013	RETURN
ISN 0014	END

```

ISN 0002      FUNCTION FCT3(Y)
ISN 0003      COMMON R,SPHT,TM,TI,SL,TS,DADT,0,TBAR
ISN 0004      COMMON FO,T,RHOSF,AZ,THCONF,AY1,AY2,AY3,AY4,AY5,TIN
ISN 0005      COMMON APPRL
ISN 0006      TR71=(3.*FO*T/(RHOSF*SPHT*R1)*Y**2.
ISN 0007      TR72=(FO*(5.*(Y**2.1)-3.*(R**2.1))/(10.*THCONF*R1)*Y**2.
ISN 0008      TR73=(2.*FO*(R**2.1)/THCONF)*Y
ISN 0009      TR74=SIN(Y*4.49/R)*EXP(AZ*AY1)/(AY1*SIN(4.49))
ISN 0010      TR75=SIN(Y*7.725/R)*EXP(AZ*AY2)/(AY2*SIN(7.725))
ISN 0011      TR76=SIN(Y*10.9/R)*EXP(AZ*AY3)/(AY3*SIN(10.9))
ISN 0012      TR77=SIN(Y*14.07/R)*EXP(AZ*AY4)/(AY4*SIN(14.07))
ISN 0013      TR78=SIN(Y*17.22/R)*EXP(AZ*AY5)/(AY5*SIN(17.22))
ISN 0014      GR1= TR74+TR75+TR76+TR77+TR78
ISN 0015      GRT=TR71+TR72-TR73*(GR1)
ISN 0016      FCT3=GRT
ISN 0017      RETURN
ISN 0018      END

```

Drop - Solid

Surface Cond. - Fixed T_I

Fuel - UO_2 (T_{IN} -2800 °C)

Radius - .01 cm

Coolant - Na (T_{COOL} -200 °C)

TIME= 0.00050

TAN THERMAL	-0.131825E 05
TAN THERMAL	-0.131776E 05
TAN THERMAL	-0.131647E 05
TAN THERMAL	-0.131239E 05
TAN THERMAL	-0.130276E 05
TAN THERMAL	-0.128202E 05
TAN THERMAL	-0.123940E 05
TAN THERMAL	-0.115572E 05
TAN THERMAL	-0.555346E 04
TAN THERMAL	-0.724721E 04
TAN THERMAL	-0.270075E 04
TAN THERMAL	0.436742E 04
TAN THERMAL	0.146803E 05
TAN THERMAL	0.287819E 05
TAN THERMAL	0.468207E 05
TAN THERMAL	0.683625E 05
TAN THERMAL	0.923081E 05
TAN THERMAL	0.116986E 06
TAN THERMAL	0.140411E 06

CF 0.00590000

CRACK DEPTH(CM).00059000	K-1 FACTCR(C)(P/13/2)	0.4465E 04
CRACK DEPTH(CM).00158000	K-1 FACTCR(C)(P/13/2)	0.4556E 04
CRACK DEPTH(CM).00257000	K-1 FACTCR(C)(P/13/2)	0.4687E 04
CRACK DEPTH(CM).00396000	K-1 FACTCR(C)(P/13/2)	0.3565E 04
CRACK DEPTH(CM).00495000	K-1 FACTCR(C)(P/13/2)	0.3060E 04
CRACK DEPTH(CM).00594000	K-1 FACTCR(C)(P/13/2)	0.2101E 04
CRACK DEPTH(CM).00693000	K-1 FACTCR(C)(P/13/2)	0.1157E 04
CRACK DEPTH(CM).00792000	K-1 FACTCR(C)(P/13/2)	0.4316E 03
CRACK DEPTH(CM).00891000	K-1 FACTCR(C)(P/13/2)	-0.1256E 03
CRACK DEPTH(CM).00990000	K-1 FACTCR(C)(P/13/2)	-0.4140E 03

Drop - Liquid

Surface Cond. - Fixed T_I

Fuel - UO_2 (T_m -2800 °C)

Radius - .005 cm

Coolant - Na (T_{COOL} -200 °C)

```
TIME= 0.0000242      S-L INTERFACE POSITION=.0046      QADT= -0.1350E 12
TAN THERMAL          -.459021E 06
TAN THERMAL          -.418624E 06
TAN THERMAL          -.375464E 06
TAN THERMAL          -.329842E 06
TAN THERMAL          -.282057E 06
TAN THERMAL          -.232380E 06
TAN THERMAL          -.181081E 06
TAN THERMAL          -.126418E 06
TAN THERMAL          -.746330E 05
TAN THERMAL          -.199742E 05
TAN THERMAL          0.353344E 05
TAN THERMAL          0.910743E 05
TAN THERMAL          0.147017E 06
TAN THERMAL          0.202975E 06
TAN THERMAL          0.258741E 06
TAN THERMAL          0.314125E 06
TAN THERMAL          0.368942E 06
TAN THERMAL          0.423015E 06
TAN THERMAL          0.476163E 06
CF          .50063158
CRACK DEPTH(CM).00006316      K-1 FACTOR(Q)(P/13/2) 0.4756E 04
CRACK DEPTH(CM).00012632      K-1 FACTOR(Q)(P/13/2) 0.4816E 04
CRACK DEPTH(CM).00018947      K-1 FACTOR(Q)(P/13/2) 0.4785E 04
CRACK DEPTH(CM).00025263      K-1 FACTOR(Q)(P/13/2) 0.4254E 04
CRACK DEPTH(CM).00031579      K-1 FACTOR(Q)(P/13/2) 0.3352E 04
CRACK DEPTH(CM).00037895      K-1 FACTOR(Q)(P/13/2) 0.2151E 04
CRACK DEPTH(CM).00044211      K-1 FACTOR(Q)(P/13/2) 0.6998E 03
CRACK DEPTH(CM).00050527      K-1 FACTOR(Q)(P/13/2) -0.9664E 03
CRACK DEPTH(CM).00056842      K-1 FACTOR(Q)(P/13/2) -0.2822E 04
CRACK DEPTH(CM).00063158      K-1 FACTOR(Q)(P/13/2) -0.4845E 04
CRACK DEPTH(CM).00069474      K-1 FACTOR(Q)(P/13/2) -0.7018E 04
```

Figure 2.1 Models for Temperature and Thermal Stress Analysis

Figure 2.2 Comparison of the Transient Numerical Solution to the Steady-State Approximation for Fixed h Surface Boundary Condition

Figure 2.3 Effect of the Different Surface Boundary Conditions for a Liquid Drop on Solidification

Figure 2.4 Effect of the Different Surface Boundary Conditions on Temperature for a Liquid Drop

Figure 2.5 Effect of the Different Surface Boundary Conditions on Temperatures for a Solid Drop

Figure 3.1 Typical Tangential Stress Profile for Liquid Drop

Figure 3.2 Typical Tangential Stress Profile for Solid Drop

Figure 3.3 The Effect of Density Change of UO_2 During Solidification for the Creation of a Void

Figure 3.4 Fracture Stress of Non-irradiated UO_2 as a Function of Temperature

Figure 4.2. Values of K_I for Progressive Crack Depth at Various Time Steps for an Initially Liquid Droplet with Fixed T_I

Figure 4.3 Values of K_I for Progressive Crack Depth at Various Time Steps for an Initially Liquid Droplet with Fixed $T_I \approx 945^\circ\text{C}$

Figure 4.4 Values of K_I as a Function of the Fixed Interface Temperature

Figure 4.5 Values of K_I for Progressive Crack Depth at Various Time Steps for an Initially Liquid Droplet with Fixed Surface Heat Transfer Coefficient

Figure 4.6 Values of K_I as a Function of Fixed Heat Transfer Coefficient

Figure 4.7 Values of K_I as a Function of the Sodium Coolant Temperature

Figure 4.8 Values of K_I for Progressive Crack Depth at Various Time Steps for a Solid Drop at Fixed $T_I = 2800^\circ\text{C}$

Figure 4.9 Values of K_I for Progressive Crack Depth at Various Time Steps for a Solid Drop at Fixed $T_{\text{IN}} = 2800^\circ\text{C}$

Figure 4.10 Values of K_{I} as a Function of the Initial Solid-Coolant Temperature Difference

Figure 4.11. Values of K_I for Progressive Crack Depth at Various Time Steps for a Solid Drop with Fixed Heat Transfer Coefficient

Figure 4.12 Values of K_I as a Function of Surface Heat Transfer Coefficient for Solid Drop

Figure 4.13 Values of K_{I} as a Function of Initial Solid-Coolant Temperature Difference

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