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Thermal Simulation of Burned Nuclear Fuel Elements

Nguyen Tuan Anh

Faculty of Energy Technology, Electric Power University,
235 Hoang Quoc Viet, Hanoi, Vietnam
E-mail: dr.tanh@gmail.com

Abstract: An adjustable description of the temperature distribution in the nuclear fuel elements is evaluated to the prediction of the lifetime behavior of these components. The impact of the fuel and coolant temperature on the neutron reaction rates provides an incentive for accurate modelling of the temperature behavior under transient as well as steady-state operating conditions. This paper is to focus on the steady-state temperature field in the fuel elements. Many of the principles applied are also useful for describing the temperature field in the structure component.

Keywords: *Nuclear fuel element; thermal performance; temperature distribution; thermal conductivity; fuel structure.*

I. INTRODUCTION

The temperature in the fuel material depends on the heat-generation rate, the fuel material properties, and the coolant and cladding temperature conditions [1]. The rate of heat generation in a fuel pin depends on the neutron slowing rates near the fuel pin and the neutron reaction rate within the fuel. In return, the neutron reaction rate depends on the fuel material (both the initial compositions and burnup level) and the moderator material and their temperatures. Hence, an exact prediction of the fuel material temperature requires simultaneous determination of the neutronic and temperature fields, although for certain conditions it is possible to decouple the two fields. Thus it is assumed that the heat-generation rate is fixed as we proceed to obtain the fuel temperature field.

Uranium dioxide (UO_2) has been used exclusively as fuel material in light-water power reactors (LWRs) [2-4]. Early liquid-metal-cooled reactors relied on plutonium as a fuel and more recently on a mixture of UO_2 and PuO_2 [5]. UO_2 used in LWRs has been marked with satisfactory chemical and irradiation tolerance [6]. This tolerance has overshadowed the disadvantages of low thermal conductivity and uranium atom density relative to other materials, e.g., the nitrides and carbides or even the metal itself. The carbides and nitrides, if proved not to swell excessively under irradiation, may be used in future reactors [7]. The low density of uranium atoms in UO_2 requires a larger core for a given amount of fissile species than if a fuel of higher uranium density were used [8]. Increase in reactor size with no increase in power raises the capital cost of the reactor. Poor thermal conductivity means that the center-line temperature of the fuel and the temperature difference between the center and the surface of the rod must be very large in order that sufficient fission heat be extracted from a unit of fuel to make electric power production economical [9]. On the other hand,

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central fuel temperatures close to the melting point have a beneficial fission-product scouring effect on the fuel.

The article is organized as follows. Temperature distribution of a typical fuel element in cylindrical geometry just startup of operating process of light water reactors is considered in Section II. Section II includes temperature distribution in restructured fuel element after operating. In Section IV, the heat conduction problem in cylindrical fuel element that have undergone some irradiation, and hence developed sintered regions, is solved by a simulation model. Finally, conclusion and outlook are given in Section V.

II. TEMPERATURE DISTRIBUTION IN CYLINDRICAL FUEL RODS

Cylindrical fuel pellets are nearly universally used as the fuel form in power reactors.

A. General Conduction Equation for Cylindrical Geometry

If the neutron flux is assumed to be uniform within the fuel pellet, the heat-generation rate can be assumed uniform. The coolant turbulent flow conditions in a fuel assembly of a pin pitch-to-diameter ratio of more than 1.2 is such that the azimuthal flow conditions ban be taken to be essentially the same around the fuel rod. The above two conditions lead to the conclusion that no significant azimuthal temperature gradients exist in the fuel pellet. Also, for a fuel pin of a length-to diameter ratio of more than 10, it is safe to neglect the axial heat transfer within the fuel relative to the radial heat transfer for most of the pin length. However, near the top and the bottom ends, axial heat conduction plays a role in determining the temperature field.

Thus the steady-state temperature distribution in a cylindrical body in which heat is generated at a volumetric rate H is governed by the heat-conduction equation:

$$\frac{1}{r}\frac{d}{dr}\left(rk\frac{dT}{dr}\right) + H = 0, \qquad (1)$$

Where the thermal conductivity k is intrinsically a function of temperature and can also depend on position because of radial porosity variations in the fuel. The value H is the volumetric heat-generation rate, which can be a function of radial position.

Many of the factors that affect both the magnitude and radial variation of H and k are time dependent. The removal of porosity due to fuel restructuring occurs in a matter of hours, and fission-gas generation causes changes on a time scale measured in weeks or months. Redistribution of fissile species can have even larger characteristic times. In general, changes in k and H due to materials transformations are so gradual that, for fuel-element operation at constant power, the heat-conduction process can be considered to be at steady-state.

Solution of equation (1) requires two boundary condition. One is the specified temperature at the surface of the fuel ($r = R$)

$$T(R) = T_s. \qquad (2)$$

The fuel rod may have a hole in the center. Irrespective of whether the central hole is purposely manufactured into the fuel pellet or whether it develops as a result of irradiation, the boundary of the void constitutes an isothermal surface of temperature T_0. Furthermore, since there is no heat generation in the gas contained in the central void, the heat flux at this surface is zero,

$$\left(\frac{dT}{dr}\right)_{r_0} = 0, \qquad (3)$$

Where r_0 is the radius of the central void.

B. Volumetric Heat-Generation Rate

The local volumetric heat-generation rate is related to the fission density by

$$H = 3.2 \times 10^{-11} \dot{F} \ \text{W/cm}^3. \quad (4)$$

The fission density is given by

$$\dot{F} = q\sigma_f N_f \Phi \quad \text{fissions cm}^{-3}\,\text{s}^{-1}, \quad (5)$$

where q is enrichment, σ_f is effective fission cross section, N_f is total number of heavy-metal atoms per unit volume, and Φ is neutron flux. In (5) the terms can change with irradiation time and vary with radius in the fuel rod. To isolate these effects, we combine it with (4) in the following manner:

$$H = (3.2 \times 10^{-11} q_0 \sigma_f N_{f0} \bar{\Phi}_0) \left(\frac{\bar{q}}{q_0}\frac{\bar{N}_f}{N_{f0}}\frac{\bar{\Phi}}{\bar{\Phi}_0}\right)\left(\frac{q}{\bar{q}}\frac{N_f}{\bar{N}_f}\frac{\Phi}{\bar{\Phi}}\right). \quad (6)$$

The first term on the right-hand side of Eq. (6) is the average volumetric heat-generation rate at startup. The second term contains the effect of burnup on the heat-generation rate. The third term contains terms describing the radial variation of quantities affecting the heat-generation rate. All are normalized to unity

$$\bar{q} = \frac{2}{R^2 - r_0^2}\int_{r_0}^{R} r\, q(r)\, dr, \quad (7a)$$

$$\bar{N}_f = \frac{2}{R^2 - r_0^2}\int_{r_0}^{R} r\, N_f(r)\, dr, \quad (7b)$$

$$\bar{\Phi} = \frac{2}{R^2 - r_0^2}\int_{r_0}^{R} r\, \Phi(r)\, dr. \quad (7c)$$

The thermal rating of a fuel rod is usually described in terms of its linear power, defined by

$$\wp = \frac{\text{power}}{\text{unit length of rod}} \quad \text{W/cm}. \quad (8)$$

The linear power varies with axial position in the fuel rod. The linear power is related to the radially averaged volumetric heat-generation rate by

$$\frac{\wp}{\pi(R^2 - r_0^2)} = \bar{H} = \frac{2}{R^2 - r_0^2}\int_{r_0}^{R} r\, H(r)\, dr. \quad (9)$$

The object of solving Eq. (1) is twofold. First, the temperature profile in a fuel rod is needed to accurately estimate the extent of materials transformations, such as swelling, gas release, sintering, and mechanical interaction between the fuel and the cladding. Second, it is important to be able to predict the maximum temperature in a fuel rod for specified linear power and fuel conditions to the melting point.

C. The Conductivity Integral

The primary impediment to direct integration of Eq. (1) is the radial and temperature variation of the thermal conductivity. Considerable progress in analyzing the thermal characteristics of a fuel rod can be made without confronting the complex behavior of k by an approach that is generally referred to as the conductivity-integral concept.

Consider first the case of a solid fuel rod with a constant volumetric heat-generation rate,

$$H = \frac{\wp}{\pi R^2}. \quad (10)$$

Equation (1) may be integrated once to yield

$$rk\frac{dT}{dr} = -\frac{1}{2}Hr^2. \quad (11)$$

The constant of integration is zero by Eq. (3) with $r_0 = 0$ for a solid rod. Integration of Eq. (11) between any position and the surface yields

$$\int_{T_s}^{T} k\, dT = \frac{1}{4}HR^2\left(1 - \frac{r^2}{R^2}\right), \quad (12)$$

or, in terms of the center temperature T_0,

$$\int_{T_s}^{T_0} k\, dT = \frac{1}{4}HR^2. \quad (13)$$

If k is constant, the solution of Eq. (11) is

$$\frac{T - T_s}{T_0 - T_s} = 1 - \frac{r^2}{R^2}. \quad (14)$$

Consider the case of an annular pellet, with a constant volumetric heat-generation rate,

$$H = \frac{\wp}{\pi(R^2 - r_0^2)}. \quad (15)$$

Eq. (1) can be integrated once to get

$$rk\frac{dT}{dr} = -\frac{1}{2}H(r^2 - r_0^2). \quad (16)$$

Integration of Eq. (16) yields

$$\int_{T_s}^{T} k\, dT = \frac{1}{4}HR^2\left[\left(1 - \frac{r^2}{R^2}\right) + \frac{r_0^2}{R^2}\ln\left(\frac{r^2}{R^2}\right)\right], \quad (17)$$

or, in terms of the void temperature T_0,

$$\int_{T_s}^{T_0} k\, dT = \frac{1}{4}HR^2\left[\left(1 - \frac{r_0^2}{R^2}\right) + \frac{r_0^2}{R^2}\ln\left(\frac{r_0^2}{R^2}\right)\right]. \quad (18)$$

Simulations of the temperature distributions will be given in Section 4.

The conductivity integral can be applied to situations where H is a function of r provided that the form of this dependence can be specified.

In a thermal reactor the heat-generation rate varies with radius because of the depression of the neutron flux in the center of the rod. The flux ratio is given by

$$\frac{\Phi(r)}{\bar{\Phi}} = \frac{\kappa R}{2I_1(\kappa R)} I_0(\kappa r), \quad (19)$$

Where I_0 and I_1 are modified Bessel functions of the first kind of zeroth and first order, respectively, and κ is the reciprocal of the neutron-diffusion length in the fuel material (typically 2 to 3 cm^{-1} in thermal reactor oxide fuel).

The other two factors in the last term of Eq. (6) are assumed to be unity, then the heat-generation rate is given by

$$H(r) = \frac{\wp}{\pi R^2}\left[\frac{\kappa R}{2I_1(\kappa R)} I_0(\kappa r)\right]. \quad (20)$$

With Eq. (20), Eq. (1) can be integrated twice with the aid of the surface and center boundary conditions. For a solid rod the result is

$$\int_{T_s}^{T_0} k\, dT = \frac{\wp}{4\pi}\left[\frac{I_0(\kappa R) - 1}{(\kappa R/2)I_1(\kappa R)}\right]. \quad (21)$$

The effect of the flux depression is to reduce the conductivity integral for a fixed linear power. For a specified fuel surface temperature, the center of the fuel rod is cooler for the case of flux depression compared to a radially uniform flux. From a heat-conduction point of view, it is advantageous to move the heat source to the periphery of the rod, which is effectively what the flux depression does. The effect is general: any phenomenon that decreases heat generation at the center of the rod reduces the central temperature.

III. TEMPERATURE DISTRIBUTION IN RESTRUCTURED FUEL

Operation of an oxide fuel material at high temperature leads to alterations of its morphology. The fuel region in which the temperature exceeds a certain sintering temperature experiences loss of porosity. In a cylindrical fuel pellet the inner region is restructured to form a void at the center, surrounded by a dense fuel region [8, 9]. In fast reactors, where the fuel may have a higher temperature near the center, restructuring was found to lead to three distinct regions [10, 11]. In the outermost ring, where no sintering (i.e., no densification) occurs, the fuel density remains equal to the original (as fabricated) density, whereas the intermediate and inner regions have densities of 95 to 97% and 98 to 99%, respectively. It should be note that most of the restructuring occurs within the first few days of operation, with slow changes afterward. In LWRs, where the fuel temperature is not as high as in liquid-metal-cooled reactors, two-region pellet restructuring may occur in the core regions operating at high powers.

In this section, temperature distributions are obtained on the assumption that the fuel element may be represented by two regions.

A. Mass Balance

From conservation of mass across a section in the fuel rod before and after restructuring, we conclude that the original mass is equal to the sum of the fuel mass in the two rings. Hence when the pellet length is assumed unchanged:

$$\pi R^2 \rho_0 = \pi(r_1^2 - r_0^2)\rho_1 + \pi(R^2 - r_1^2)\rho_2. \quad (22)$$

However, the initial density ρ_0 is equal to ρ_2, so that an expression for r_0 can be obtained from Eq. (22) as,

$$r_0^2 = \frac{\rho_1 - \rho_2}{\rho_1} r_1^2. \quad (23)$$

B. Power Density Relations

For a uniform neutron flux the heat-generation density is proportional to the mass density

$$H_1 = \frac{\rho_1}{\rho_2} H_2 \,. \quad (24)$$

The density ratios in these equations represent the atom-density ratio $N_f(r)/N_{f0}$ in Eq. (6) for the two regions where fuel sintering has occurred. The enrichment and flux ratios in Eq. (6) are assumed to be unity for this calculation.

The linear power is given by the summation of the heat-generation rate in the two rings. Therefore, the linear power in the restructured fuel $\wp$ is given by

$$\wp = H_2\, \pi(R^2 - r_1^2) + H_1\, \pi(r_1^2 - r_0^2) \quad (25a)$$

or

$$\wp = H_2 \left[\pi(R^2 - r_1^2) + \frac{\rho_1}{\rho_0}\, \pi(r_1^2 - r_0^2)\right] \quad (25b)$$

Combining Eqs. (22) and (25b), we obtain

$$\wp = H_2\, \pi R^2 \quad (26)$$

That is, the linear power in the as-fabricated region can be obtained from the assumption that the mass is uniformly distributed in the fuel pellet. It is equivalent to expecting the linear power in the outer region not to be affected by the redistribution of the fuel within the other zone.

C. Two-zone Sintering

Integration of the heat-conduction equation (1) for the region 2 once yields

$$r k_2 \frac{dT}{dr} = -\frac{1}{2} H_2 r^2. \quad (27)$$

Where k_2 is the thermal conductivity of the fuel for temperature between T_s and T_1 and for the porosity of the as-fabricated fuel.

A second integration yields

$$\int_{T_s}^{T} k_2\, dT = \frac{\wp}{4\pi}\left(1 - \frac{r^2}{R^2}\right), \quad (28a)$$

or, in term of the temperature T_1,

$$\int_{T_s}^{T_1} k_2\, dT = \frac{\wp}{4\pi}\left(1 - \frac{r_1^2}{R^2}\right), \quad (28b)$$

Similarly, the first and the second integrals of the heat-conduction equation in the region 1 are

$$r k_1 \frac{dT}{dr} = -\frac{1}{2} H_1 (r^2 - r_0^2). \quad (29)$$

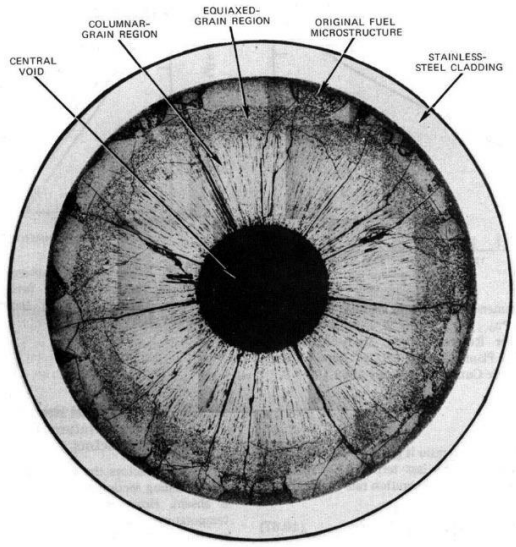
$$\int_{T_0}^{T} k_1\, dT = \frac{\wp}{4\pi}\frac{\rho_1}{\rho_2}\frac{r_0^2}{R^2}\left[\left(1 - \frac{r^2}{r_0^2}\right) + \ln\left(\frac{r^2}{r_0^2}\right)\right]. \quad (30a)$$

or, in terms of the temperature T_1,

$$\int_{T_1}^{T_0} k_1\, dT = \frac{\wp}{4\pi}\frac{\rho_1}{\rho_2}\frac{r_1^2}{R^2}\left[\left(1 - \frac{r_0^2}{r_1^2}\right) + \frac{r_0^2}{r_1^2}\ln\left(\frac{r_0^2}{r_1^2}\right)\right]. \quad (30b)$$

The temperature distribution in the rod can be obtained as follows. Assume that the fuel surface temperature T_s, the linear power $\wp$, and the density of the fabricated fuel ρ_2/ρ_s have been specified. The properties of the region (T_1, ρ_1/ρ_s) are also presumed to be known. Equations (23), (28b), and (30b) provide three equations from which the three unknowns r_0/R, r_1/R, and T_0 can be determined. First, r_1/R is

determined by solving Eq. (28b). The radius of the central void is then obtained from Eq. (23). Next, the conductivity integral for the inner zone is given by Eq. (30b). Finally, the values of the conductivity integral obtained from the measurements of several laboratories is used to get T_0.



The method just described fixes the radius and temperature of the central void surface and the locations of the boundaries between the two regions, each of which is associated with a specific temperature. The temperature profile between these anchor points can be obtained from Eqs. (28a) and (30a). Simulations of the temperature distributions will be given in Section III [12].

IV. SIMULATION OF TEMPERATURE DISTRIBUTION

Figures 1a and 1b show simulations of typical temperature distributions just at startup. The slops of the temperature distributions are continuous from the void radius r_0 to the fuel surface radius R. r_0, T_0, and T_s can be varied to obtain any stage.

Figures 2a and 2b show simulations of typical temperature distributions just after fuel restructuring has occurred. The slops of the temperature distributions are discontinuous at the boundaries separating the various regions because the thermal conductivities, according to the model, change discontinuously at r_1. As expected, the maximum temperature attained by the fuel decreases substantially as a result of densification and central-void formation. The net effect of these processes is to move the nuclear heat source further toward the periphery of the rod than is the case in the solid rod of as-fabricated fuel. Such a displacement effectively reduces the path length over which heat must be conducted; so a given heat flux can be sustained with a smaller temperature difference. The higher thermal conductivity in region 1 which results from densification also act to reduce fuel temperature.

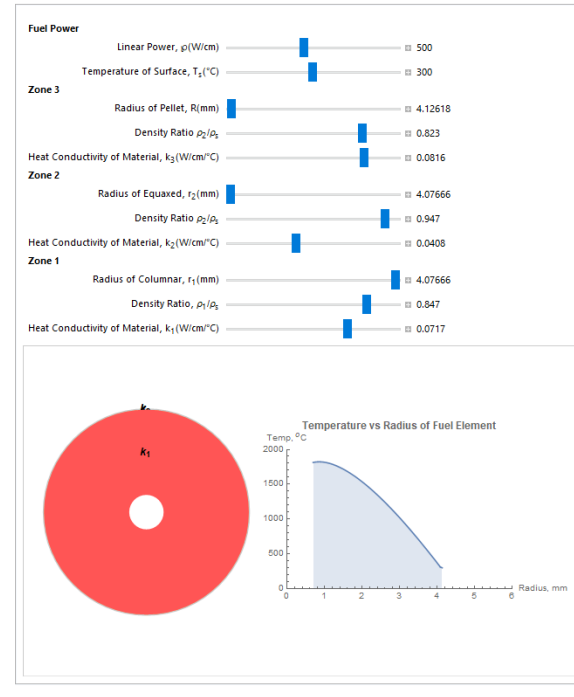


Fig. 1a. Simulations of typical temperature distributions just at startup. The slops of the temperature distributions are continuous. Parameters r_0, T_0, and k can be varied to obtain any stage

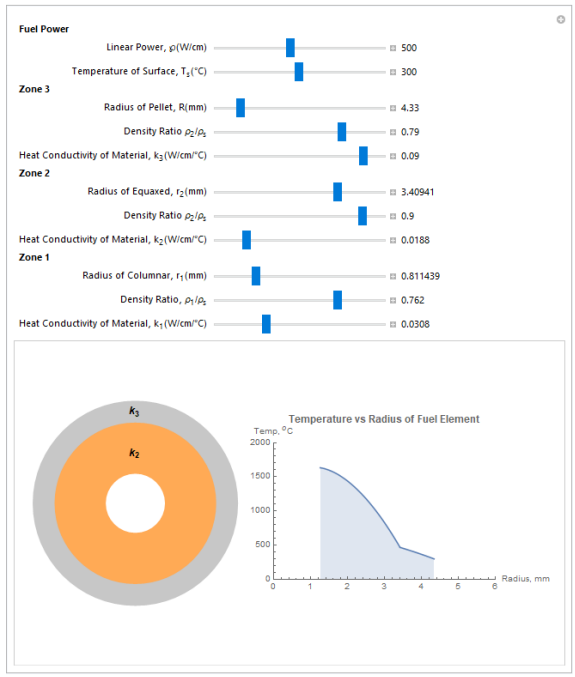


Fig. 1b. Simulations of typical temperature distributions just at startup from the void radius r_0 to the fuel surface radius R

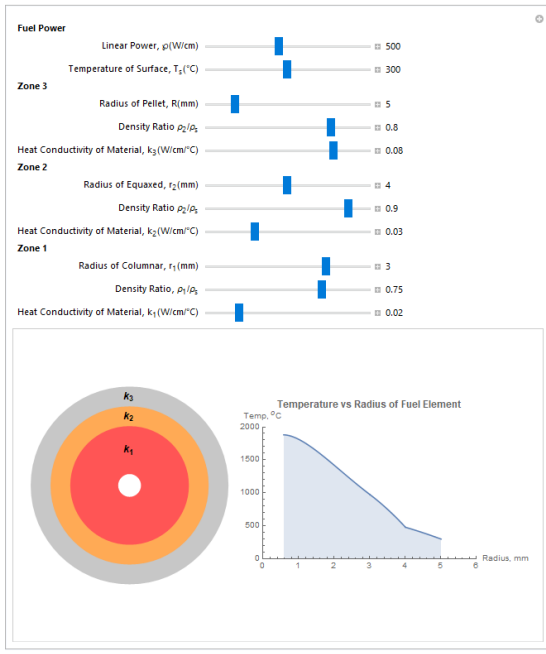


Fig. 2a. Simulations of typical temperature distributions just after fuel restructuring has occurred. The slops of the temperature distributions are discontinuous at the boundaries separating the various regions because the thermal conductivities change discontinuously at r_1. Parameters r_0, T_0, ρ_1/ρ_s, ρ_2/ρ_s, and k_1 and k_2 can be varied to obtain any stage

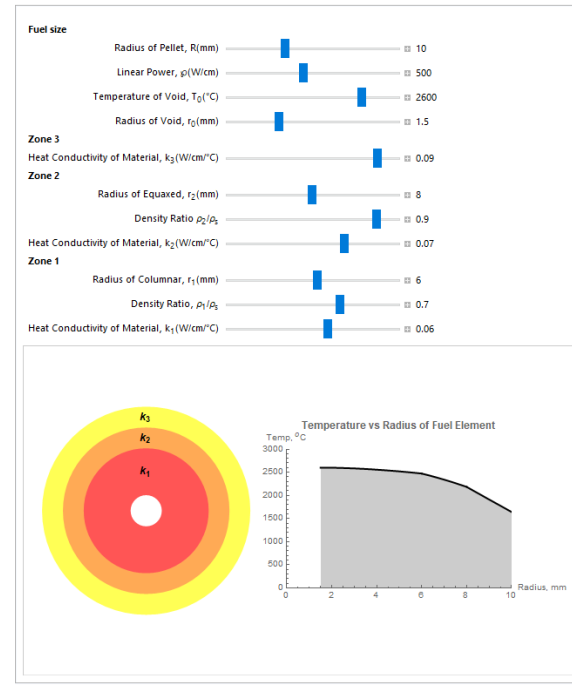


Fig. 2b. Simulations of typical temperature distributions in with other values of parameters

V. THE OUTLOOK AND CONCLUSIONS

Solutions to the heat-conduction equation, Eq. (1), which incorporate many of the features must be accomplished by finite-difference techniques. Computer simulations have been released for this purpose.

If the coolant temperature at each axial location is known from the specified axial variation in the linear power and the thermal-hydraulic characteristics of the coolant, a complete description of the radial and axial fuel temperature distribution and fuel restructuring can be obtained.

The methods described in this article for determining the temperature profile in a high rated fuel rod are better than the assumption of a parabolic temperature distribution, but they do not consider many important features of fuel thermal performance [13-15]. A better calculation and simulation should include:

1. Differential thermal expansion of the

fuel and the consequent displacement of the hot, plastic core region 1 toward the center. This effect tends to reduce the size of the central void.

2. Axial fuel displacement (due, for example, to vapor transport of fuel material within the central void).

3. Cracking of the fuel due to thermal stresses. Radial cracks probably do not affect the temperature profile, as much as circumferential cracks, which act as gas-filled gaps.

4. The dynamic nature of the fuel restructuring process. The zone boundaries r_0 and r_1 are in reality functions of irradiation time.

5. The generation of porosity by fission-gas bubbles, expansion due to solid fission products, and reduction porosity by hydrostatic pressure (hot pressing).

6. The continuous rather than the discrete nature of the porosity variation with radius.

7. The role of thermal expansion, fuel swelling, and cladding swelling in changing the fuel-cladding gap conductance, which causes the fuel surface temperature to vary with irradiation time even through the coolant temperature at the particular axial location is constant.

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