A SIMPLE, REASONABLY ACCURATE MODEL FOR CALCULATING STRESSES IN THE LAYERS OF COATED FUEL PARTICLES DURING IRRADIATION

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SUMMARY

Explicit analytical expressions have been developed which enable the maximum stresses in the various layers of a triplex coated fuel particle (comprising coatings of inner pyrocarbon, silicon carbide and outer pyrocarbon respectively) to be calculated during the course of an isothermal irradiation, in terms of the physical properties of the layers and the inner and outer pressures acting on the coatings. The accuracy of these expressions is typically 1-2%.

In order to derive these relations it was assumed that with the exception of the dimensional change rates under irradiation all materials' properties relating to the layers were cubic and independent of neutron dose; also that the deformation of the silicon carbide layer due to elastic and creep strains may be neglected.

The quoted analytical equations, which enable stresses to be calculated very easily by hand, assume that for the pyrocarbon layers the dimensional change rates due to irradiation are the same at all points within a particular layer and are independent of neutron dose; also that the silicon carbide dimensional change rates may be neglected. However it is shown that by suitably modifying the values of the dimensional change rates used in the calculations any or all of these three assumptions may be eliminated. As a result the model can adequately handle any dimensional change data it is presented with; for example it can deal with situations for which pyrocarbon layers comprise material with different density, as is the case with inner pyrocarbon layers which are deposited from methane.

A physical appreciation of these rather formal mathematical relationships may be gained by converting them into a form which is valid when layers are so thin that terms in $(t/r)^2$ and higher powers of t/r, where t is the thickness and r the mean radius, may be neglected.

The analytical model also enables the relative importance of the various input variables on the stresses to be readily assessed quantitatively. An example of this is the relative contribution to stresses of radial compared with tangential dimensional change rates of a specific pyrocarbon layer.

The model can be readily extended to give also the radial displacements of the two free pyrocarbon surfaces during the course of an irradiation.

1. Introduction

A number of mathematical models to describe the mechanical performance of coated fuel particles during irradiation have been developed (Hick et al. [1]). Generally their complexity demands that the solution be obtained by computer. By contrast the aims of the present paper is to develop a simple, but reasonably accurate analytical solution. Such a model is useful for gaining a greater physical appreciation of the problem, identifying the relative importance of the various items of input data, checking the correctness of computer codes based on other models, and, when these are not available, calculating particle endurances by hand.

We shall only consider here those particles whose fission products are retained by three layers, namely a silicon carbide layer sandwiched between an inner and an outer pyrocarbon layer. These will be denoted subsequently by the abbreviations SiC, IPyC and OPyC respectively. The specifications of such a particle, approximating to the type of particle which has been under consideration in the U.K. in recent years, and which will be called subsequently the model particle, are given in table I. Since metallographic examination shows that for such particles the kernel is debonded from the buffer layer, and the buffer undergoes severe damage during the irradiation (assumed here to be isothermal), we shall assume that neither directly affects the particle performance.

We shall confine our attention in this paper to relating the physical properties of the various layers and the inner and outer pressures with the maximum stresses and strains in each layer. This will enable the possibility of failure of a layer by one of two alternative failure mechanisms, namely as a result of either the fracture stress or the creep ductility limit being attained, to be considered. In order to use the analytical relationships derived here to calculate particle endurances the relationships between burn-up and inner and outer pressures must be known. The outer pressure, which is generally the smaller, can usually be estimated to tolerable accuracy. Inner pressures, created by the gas released due to fission, can also be calculated to a fair accuracy provided that the change in internal voidage due to radiation dimensional changes of the IPyC layer and the increase in solid volume of the kernel due to the build-up of solid fission products are allowed for. For example, for a model particle given an irradiation dose typical of a U.K. design high temperature reactor, the gas pressure was found to be overestimated by about 2% using this calculation procedure. If a higher accuracy is required an allowance for volume changes due to the creep of the IPyC layer (eq. (11)) may be made.

2. Basic Assumptions and Theory

The assumptions which are basic to the present model are that (i) all layers possess spherical symmetry, (ii) all materials' properties relating to layers, with the exception of dimensional change rates due to irradiation, are cubic and independent of neutron dose, and (iii) the deformation of the SiC layer due to elastic and creep strains is negligibly small. Assumption (i) is basic to all previous models, while (ii) would seem to be justifiable on the basis of current knowledge. Assumption (iii) implies that the radiation creep constant of silicon carbide is negligibly small and the elastic constant extremely large compared with the corresponding values of pyrocarbon (abbreviated subsequently to PyC). The validity of this assumption was tested with the aid of an accurate computer code based on the

Walther [2] model. For the model particle it was found that only small fractional errors in the stresses (~ 1–2%) or alternatively, if stress models are low, small absolute errors (~ 1–2 MN/m^2) resulted from the use of approximation (iii).

Initially we shall make three additional assumptions and then show subsequently how the derived results are modified when they are eliminated. These assumptions are (a) the radiation induced dimensional change rate of SiC is zero; (b) dimensional change rates in each PyC layer are independent of radial position within the layer; (c) dimensional change rates and inner and outer pressures are independent of neutron dose, so that all stresses within layers are dose independent.

The equations of compatibility are

$$\dot{\varepsilon}_1 = \frac{\dot{u}}{x} \tag{1}$$

and

$$\dot{\varepsilon}_3 = \dot{u}' \tag{2}$$

where ε denotes the overall strain at a point whose radial co-ordinate within a particular layer is x, u is the radial displacement, subscripts 1 and 3 refer to the tangential and radial directions, and the dot and prime denote differentiation with respect to neutron dose and x respectively.

The relations between the rates of strain, radiation induced dimensional changes and creep are

$$\dot{\varepsilon}_1 = \dot{g}_1 + K(1-\nu)\sigma_1 - K\nu\sigma_3 \tag{3}$$

and

$$\dot{\varepsilon}_3 = \dot{g}_3 + K\sigma_3 - 2K\nu\sigma_1 \tag{4}$$

where g is the fractional dimensional change due to irradiation, σ the stress, K the uniaxial creep constant and ν Poisson's ratio in creep. Following previous workers we have assumed that radiation creep is directly proportional to both neutron dose and stress and that thermal creep may be neglected. Note also that because stresses are independent of dose eqs. (3) and (4) do not include terms involving the elastic constants.

σ_1 and σ_3 are related by the equation of equilibrium

$$\sigma_1 = \sigma_3 + \tfrac{1}{2}x\sigma_3'. \tag{5}$$

Elimination of ε_1, ε_3, u and σ_1 from eqs. (1)–(5) results in the basic differential equation in σ_3

$$x^2\sigma_3'' + 4x\sigma_3' + \frac{2\Delta\dot{g}}{K(1-\nu)} = 0 \tag{6}$$

where $\Delta\dot{g} = \dot{g}_1 - \dot{g}_3$. The solution is

$$\sigma_3 = \frac{A}{x^3} - \frac{2\Delta\dot{g}}{3K(1-\nu)}\ln x + B \tag{7}$$

where A and B are constants of integration whose values are determined by the boundary conditions for the layer. σ_1 may then be derived from eq. (5) and $\dot{u}$ from a relationship derived from eqs. (1), (3) and (5)

$$\frac{\dot{u}}{x} = \dot{g}_1 + K(1-2\nu)\sigma_3 + \tfrac{1}{2}xK(1-\nu)\sigma_3'. \qquad (8)$$

3. Analytical Expressions for the Maximum Tangential Stresses and Strain Rates in each layer

For the pyrocarbon layers the maximum tangential stresses and strain rates will occur at either the inner or outer surface. For the SiC layer the maximum stress in all situations for which fracture is possible occurs at the inner surface. Also, in accordance with assumptions (iii) and (a) above, the strain rate in the SiC layer is zero. Again, owing to the continuity of radial displacements at boundaries, at the outer surface of the IPyC and the inner surface of the OPyC layer $\dot{\varepsilon}_1 = 0$. Accordingly we shall quote formulae for tangential stresses at both surfaces and the tangential strain rate at the free surface for each PyC layer, and also for the tangential stress at the inner surface of the SiC layer.

For the calculation of stresses and strain rates in the IPyC layer, the two boundary conditions are $\sigma_3(a) = -P$ (continuity of radial stresses at the free surface) and $\dot{u}(b) = 0$ (continuity of displacements at the interface), where P is the internal gas pressure and, for the layer under consideration, a and b denote the values of x at the inner and outer surface respectively. For the OPyC layer the boundary conditions are

$$\dot{u}(a) = 0 \text{ and } \sigma_3(b) = -\Pi,$$

where Π is the outer pressure acting on the particle.

The tangential stresses at the inner and outer surfaces of the IPyC layer are given by

$$\sigma_1(a) = -\frac{9\dot{g}_1 m(1-\nu) - \Delta\dot{g}[(1+\nu)(m-1) + 2(1-2\nu)m \ln m]}{3K(1-\nu)[2m(1-2\nu) + (1+\nu)]} - \frac{(1+\nu) - m(1-2\nu)}{2m(1-2\nu) + (1+\nu)} P \qquad (9)$$

and

$$\sigma_1(b) = -\frac{3\dot{g}_1(1-\nu)(2m+1) - 2\Delta\dot{g}\nu(m-1-\ln m) + 9\nu(1-\nu)KP}{3K(1-\nu)[2m(1-2\nu) + (1+\nu)]} \qquad (10)$$

respectively, where $m = \left(\frac{b}{a}\right)^3$. Note that here and hereafter the variables $\dot{g}_1$, $\Delta\dot{g}$, K, ν and m in formulae which define stresses and strain rates in a particular PyC layer relate specifically to that layer. The tangential strain rate at the inner surface is

$$\dot{\varepsilon}_1(a) = \dot{g}_1 - \frac{9\dot{g}_1 m(1-\nu) - \Delta\dot{g}[(1+\nu)(m-1) + 2(1-2\nu)m\ln m] - 3(1+\nu)(1-2\nu)(m-1)KP}{3[2m(1-2\nu) + (1+\nu)]} \qquad (11)$$

Considering now the OPyC layer, the tangential stresses at the inner and outer surface and the tangential strain rate at the outer surface are given by

$$\sigma_1(a) = -\frac{3\dot{g}_1(1-\nu)(m+2) + 2\Delta\dot{g}\nu(m-1-m\ln m) + 9m\nu(1-\nu)K\Pi}{3K(1-\nu)[m(1+\nu) + 2(1-2\nu)]}, \qquad (12)$$

$$\sigma_1(b) = -\frac{9\dot{g}_1(1-\nu) + \Delta\dot{g}[(1+\nu)(m-1) + 2(1-2\nu)\ln m]}{3K(1-\nu)[m(1+\nu) + 2(1-2\nu)]} - \frac{m(1+\nu) - (1-2\nu)}{m(1+\nu) + 2(1-2\nu)}\Pi, \qquad (13)$$

and

$$\dot{\varepsilon}_1(b) = \dot{g}_1 - \frac{9\dot{g}_1(1-\nu) + \Delta\dot{g}[(1+\nu)(m-1) + 2(1-2\nu)\ln m] + 3(1+\nu)(1-2\nu)(m-1)K\Pi}{3[m(1+\nu) + 2(1-2\nu)]} \tag{14}$$

respectively.

Turning now to the SiC layer the tangential stress at the inner surface may be expressed by means of thick shell theory (Timoshenko and Goodier [3]) in terms of the radial stress acting on its two surfaces; bearing in mind the continuity of radial stresses at the two interfaces, the radial stresses at the SiC inner and outer surfaces may be replaced by the radial stresses at the outer surface of the IPyC layer and the inner surface of the OPyC layer respectively to give

$$\sigma_{1s}(a) = \frac{3m_s\sigma_{3o}(a) - (2+m_s)\sigma_{3i}(b)}{2(m_s-1)} \tag{15}$$

where the subscripts i, o and s denote IPyC, OPyC and SiC respectively. Finally we require expressions for the radial stress appearing in eq. (15). At the outer surface of the IPyC layer this is

$$\sigma_3(b) = -\frac{6\dot{g}_1(m-1) - 2\Delta\dot{g}(m-1-\ln m) + 9(1-\nu)KP}{3K[2m(1-2\nu) + (1+\nu)]} \tag{16}$$

and at the inner surface of the OPyC layer

$$\sigma_3(a) = \frac{6\dot{g}_1(m-1) - 2\Delta\dot{g}(m-1-m\ln m) - 9m(1-\nu)K\Pi}{3K[m(1+\nu) + 2(1-2\nu)]}. \tag{17}$$

4. The Effect on the Analytical Expressions of Eliminating some Simplifying Assumptions

The effect of eliminating assumptions (a) (b) and (c) of section 1 on the analytical expressions is now considered.

Consider first the situation when the dimensional change rates of the SiC layer are no longer zero. Assuming that these dimensional changes are isotropic the only modification required of the various expressions is to replace the variable $\dot{g}_1$ by $(\dot{g}_1-\dot{g}_s)$ where $\dot{g}_s$ is the dimensional change rate of SiC. The only exceptions to this rule occur in eqs. (11) and (14) where the first term, $\dot{g}_1$, remains unchanged.

Let us now consider the case when the dimensional change rates of pyrocarbon within a layer is a function of the radial position. Equation (6) is now modified to

$$x^2\sigma_3'' + 4x\sigma_3' + \frac{2}{K(1-\nu)}(\Delta\dot{g} + \dot{g}_1'x) = 0 \tag{18}$$

and the solution involves certain integrations of the dimensional change rates over the thickness of the layer. Let us define

$$\overline{\dot{g}_v} = \frac{3\int_a^b (2\dot{g}_1 + \dot{g}_3)x^2 dx}{b^3 - a^3} \tag{19}$$

and

$$\overline{\Delta\dot{g}} = \frac{\int_a^b \frac{\Delta\dot{g}}{x} dx}{\ln\frac{b}{a}} \tag{20}$$

Now it may be shown that in order to allow for variations in dimensional change rates with radius it is necessary to formulate two sets of general rules for the modification of the analytical expressions, according to whether they relate to the inner or outer surface of a PyC layer.

Considering first those equations which define stresses or strain rates at an inner surface (i.e. eqs. (9), (11), (12) and (17)) the variable $\dot{g}_1$ must be re-defined as its value at the inner surface of the layer, i.e. $\dot{g}_1(a)$. Terms in $\Delta\dot{g}$ must be separated into two lots; for those whose coefficients include the expression mln m, $\Delta\dot{g}$ must be replaced by $\overline{\Delta\dot{g}}$; for the remaining terms $\Delta\dot{g}$ must be replaced by $(3\dot{g}_1(a) - \dot{g}_v)$.

For those equations which define stresses or strain rates at an outer surface (i.e. eqs. (10), (13), (14) and (16)) $\dot{g}_1$ must be replaced by $\dot{g}_1(b)$; $\Delta\dot{g}$ must be replaced by $\overline{\Delta\dot{g}}$ in the case of those terms whose coefficients include the factor ln m, while for the remaining terms $\Delta\dot{g}$ must be replaced by $(3\dot{g}_1(b) - \overline{\dot{g}_v})$.

Finally let us consider the situation when the dimensional change rates and the inner and outer pressures are a function of neutron dose. In this case stresses and strain rates will be dose dependent and additional terms involving the elastic constants are now required. Eq. (6) is modified to read

$$x^2\, F\sigma_3'' + 4x\, F\sigma_3' + \frac{2\overline{\Delta\dot{g}}}{K(1-\nu)} = 0 \qquad (21)$$

where F is an operator defined as

$$F(\gamma) = \left[1 + \frac{(1-\mu)}{(1-\nu)EK} \cdot \frac{\partial}{\partial\gamma} \right] \equiv \left[1 + \frac{1}{C}\frac{\partial}{\partial\gamma} \right] ; \qquad (22)$$

E is the elastic constant of the layer and μ its Poisson's ratio, while γ is the neutron dose variable. Starting now from eq. (21) rather than eq. (6) analogous analytical expressions for stresses and strain rates may be derived provided that a term which is proportional to $(\nu-\mu)$ may be omitted. With the help of computer calculations, using the model particle, it was found that in all cases of practical interest the error in omitting this term was less than 1%, i.e. within the overall accuracy of the model.

Making this approximation then, it was found that the only modification required to the analytical expressions was to add a ˆ to all variables $\dot{g}_1$ and $\Delta\dot{g}$. This circumflex is defined by the relation

$$\hat{y} = y - \frac{\dot{y}}{C} + \frac{\ddot{y}}{C^2} - \dots \qquad (23)$$

where y is a dummy variable. The only exception to this general rule occurs in the strain rate eqs. (11) and (14), for which the first term, $\dot{g}_1$, remains unaffected.

In conclusion, although these three refinements to the analytical relations have been discussed separately in this section, they may also be employed simultaneously since they are independent of each other.

5. Discussion

A greater physical understanding of the analytical relations may be obtained by reducing them to expressions which are valid when layers are very thin. This may be achieved by expressing them in a power series in (m−1), dropping all terms of higher order than the first, and replacing (m−1) by $\frac{3t}{r}$, where t is the thickness and r the mean radius of the layer. For example eq. (16) reduces to

$$\sigma_3(b) \approx -\frac{[\dot{g}_1 - (1-2\nu)KP]}{K(1-\nu)} \cdot \frac{2t}{r} - P. \tag{24}$$

Eq. (24) is analogous to the expression derived from surface tension theory for the gas pressure inside a soap bubble, since $-\frac{[\dot{g}_1 - (1-2\nu)KP]}{K(1-\nu)}$ is simply the tangential stress in the layer due to the tangential dimensional change rate. Similarly eq. (11) reduces to

$$\dot{u}(a) \approx -t[\dot{g}_3 - (1-2\nu)KP] - t \cdot 2\nu K \cdot \frac{[\dot{g}_1 - (1-2\nu)KP]}{K(1-\nu)} \tag{25}$$

The two terms of eq. (25) have been written in a form to demonstrate that they represent the displacement rates due to dimensional changes in the radial and tangential directions respectively.

The assessment of whether a PyC layer will fail due to the creep ductility limit having been reached involves the evaluation of the creep strain, $(\varepsilon_1 - g_1)$, at the two surfaces. For those surfaces adjacent to the SiC layer this is obtained immediately since $\varepsilon_1 = 0$. For the free surfaces eqs. (11) and (14) must be integrated up to the dose under consideration. $\dot{g}_1$ and $\Delta\dot{g}$ in these equations are then simply converted into g_1 and Δg respectively. In order to integrate the inner and outer pressures over neutron dose we may note that these particular terms are normally about an order of magnitude less than the remaining terms in each expression. As a result only an approximate relationship between pressure and dose is necessary if the tangential strain is to be calculated to an accuracy of 1–2%.

As an example of the application of the analytical expressions, let us consider the maximum tangential stress in the SiC layer of the model particle and suppose that the dimensional change rates are constant throughout the IPyC layer. By means of eqs. (15)–(17) it may be shown that

$$\sigma_{1s}(a) = 2.446\frac{\dot{g}_{1o}}{K_o} + 0.126\frac{\Delta\dot{g}_o}{K_o} + 3.702\frac{\dot{g}_{1i}}{K_i} - 0.240\frac{\Delta\dot{g}_i}{K_i} + 6.425P - 8.655\Pi. \tag{26}$$

Since in practice values of $\dot{g}_1$ and $\dot{g}_3$ for a particular type of PyC differ by less than an order of magnitude we can appreciate from eq. (26) that the contribution from the $\Delta\dot{g}$ term for each PyC layer is always significantly smaller than that from the corresponding $\dot{g}_1$ term.

In order to derive eq. (26) it was assumed that $\nu = 0.40$. As an example of how the analytical model demonstrates the effect on particle endurance of variations in the input data let us suppose that $\nu = 0.35$. The equation now becomes

$$\sigma_{1s}(a) = 2.311\frac{\dot{g}_{1o}}{K_o} + 0.119\frac{\Delta\dot{g}_o}{K_o} + 3.287\frac{\dot{g}_{1i}}{K_i} - 0.213\frac{\Delta\dot{g}_i}{K_i} + 6.179P - 8.859\Pi. \tag{27}$$

Comparing eqs. (26) and (27) we see that decreasing ν from 0.40 to 0.35 results in the SiC layer being less protected from failure due to the shrinkage under irradiation of the PyC layers, but receiving greater protection from the external pressure; also a given internal pressure creates a smaller tangential stress component.

When allowance is made for the fact that the IPyC layer of the model particle comprises two PyC layers of different densities eq. (26) must be modified so that $\dot{g}_{1i}$ refers to the material of density 1.7 gm/c.c., i.e. $\dot{g}_{1i}(b)$, while the term in $\Delta\dot{g}_i$ is transformed thus:

$$- 0.240 \frac{\Delta\dot{g}_i}{K_i} \longrightarrow - 1.234 \frac{[3\dot{g}_{1i}(b) - \overline{\dot{g}_{vi}}]}{K_i} + 0.994 \frac{\overline{\Delta\dot{g}_i}}{K_i}$$

This example illustrates the conclusion that normally, for a PyC layer within which dimensional change rates vary with radius, stresses at a surface are governed largely by the $\dot{g}_1$ value at that particular surface. (In the example given here the radial stress at the outer surface of the IPyC layer is involved.)

It may also be noted that in the thin shell approximation $\overline{\dot{g}_v}$ and $\overline{\Delta\dot{g}}$ are simply the arithmetic means over the coating thickness of $(2\dot{g}_1 + \dot{g}_3)$ and $\Delta\dot{g}$ respectively.

In all the examples given in this section we ought really to have added a circumflex to all the g variables to allow for the fact that in general dimensional change rates are a function of dose. In many practical cases however it was found that the effect of this refinement is extremely small (< 1%) and may therefore be neglected.

Table I. Specifications of the Model Particle

Layer	Radius of inner and outer surface μm	Comments
Kernel	– 400	Material = UO_2, 5% enriched. Initial porosity = 22.5%.
Buffer	400 435	Assumed to possess no mechanical strength. Permeable to gas; porosity = 50%.
IPyC	435 500	Comprises a seal layer, thickness = 20 μm, density = 1.6 gm/cc. and higher density layer, thickness = 45 μm, density = 1.7 gm/cc. Deposited from methane.
SiC	500 535	
OPyC	535 590	Density = 1.8 gm/cc. Deposited from methane.

References

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