

COMTA — A COMPUTER CODE FOR FUEL MECHANICAL AND THERMAL ANALYSIS

S. BASU, S. S. SAWHNEY, A. K. ANAND,
K. ANANTHARAMAN, S. K. MEHTA

*Reactor Engineering Division, Bhabha Atomic Research Centre,
Trombay, Bombay 400 085, India*

Summary

COMTA is a generalised computer code for integrity analysis of the free standing fuel cladding, with natural UO_2 or mixed oxide fuel pellets. Thermal and Mechanical analysis is done simultaneously for any power history of the fuel pin.

For analysis, the fuel cladding is assumed to be axisymmetric and is subjected to axisymmetric load due to contact pressure, gas pressure, coolant pressure and thermal loads. Axial variation of load is neglected and creep and plasticity are assumed to occur at constant volume. The pellet is assumed to be made of concentric annuli. The fission gas release integral is dependent on the temperature and the power produced in each annulus.

To calculate the temperature distribution in the fuel pin, the variation of bulk coolant temperature is given as an input to the code. Gap conductance is calculated at every time step, considering fuel densification, fuel relocation and gap closure, filler gas dilution by released fission gas, gap closure by expansion and irradiation swelling. Overall gap conductance is contributed by heat transfer due to the three modes; conduction convection and radiation as per modified Ross and Stoute model. Equilibrium equations, compatibility equations, stress strain relationships (including thermal strains and permanent strains due to creep and plasticity) are used to obtain triaxial stresses and strains. Thermal strain is assumed to be zero at hot zero power condition. The boundary conditions are obtained for radial stresses at outside and inside surfaces by making these equal to coolant pressure and internal pressure respectively. A multi-mechanism creep model which accounts for thermal and irradiation creep is used to calculate the overall creep rate. Effective plastic strain is a function of effective stress and material constants.

For experimental verification of the computer code an irradiation programme is in progress in a thermal reactor in-pile loop at BARC. The code has been commissioned and is being used to study fuel pins with various types of power histories. The results of analysis of two fuel pins operating with same power history is given.

1.0 Introduction:

COMTA is a generalised computer code for integrity analysis of free standing cladding with pelletised fuel for thermal reactors. It is possible to use the code for both design and analysis of fuel pins with uranium oxide and mixed oxide fuel pellets. Thermal and mechanical analysis is done simultaneously for any power history of the fuel pin.

2.0 The Analytical Model:

2.1 Basic assumptions :

The fuel cladding is assumed to be axisymmetric (ovality is not accounted for) and is subjected to axisymmetric load due to coolant pressure, gas pressure, contact pressure and thermal loads. The calculations are performed far enough from the ends (at peak heat flux regions), so that the discontinuity effects are negligible. Axial variation of thermal and contact loads are considered to be negligible. Creep and plastic deformations are assumed to occur at constant volume. The fuel pellets are assumed to be made by concentric annuli and the fission gas release integral is dependent on the temperature and power produced in each annulus.

2.2 Calculations for temperature distribution:

Variation of bulk coolant temperature with heat flux and variation of heat transfer coefficients with power are taken as inputs to the code. Thermal conductivity of fuel pellets are dependent on the average temperature in the various annuli. The temperature dependent relationship for thermal conductivity of pellets, based on a reference density, is modified to account for the actual density of the annuli.

Gap conductance is calculated at every iteration for the three heat transfer modes based on modified Ross and Stoute model (Ref.1 & 2). Gap conductance due to solid-solid contact is dependent on hardness of contact surfaces, contact pressure, surface roughnesses, harmonic mean thermal conductivity of the fuel and clad. Convective gap conductance is dependent on composition of gas mixture, surface roughnesses, temperature jump distance and fuel-clad gap. The thermal conductivity of the gas mixture is dependent on the proportion of various gases and are temperature dependent functions. Contribution due to radiation heat transfer in gap conductance is also accounted for. Fuel volume is dependent on thermal expansion, irradiation swelling, fuel densification (which depends on grain growth rate constant, volumetric fission rate, irradiation induced diffusivity etc.) and fuel relocation (initially a constant and then dependent on exposure). Fission gas pressure is calculated by assuming generation to be 0.3 gas atoms/fission and release to be 4%, for those annuli with temperature below 1650°C and 100%, for those annuli with temperature above 1650°C. Other material properties like Poisson's ratio (ν), Young's Modulus (E), thermal conductivity, coefficient of expansion (α) are taken as temperature dependent functions.

2.3 Calculations for Stresses and Strains:

As the three normal components of stresses and the three longitudinal components of the total strain differ from zero and are functions of the radial coordinates only, the equilibrium equation in radial direction is given by

$$\frac{d\sigma_r}{dr} + \frac{\sigma_r - \sigma_\theta}{r} = 0 \quad \dots (1)$$

where σ_r, σ_θ are the stresses in the radial and circumferential direction and r is the radius.

The continuity equations and stress-strain relations; accounting for thermal, elastic, plastic and creep strains; are as follows :

$$\epsilon_r = \frac{du}{dr}, \quad \epsilon_\theta = \frac{u}{r}, \quad \epsilon_z = A_3 \quad \dots (2)$$

and
$$\epsilon_r = \frac{1}{E} [\sigma_r - \nu (\sigma_\theta + \sigma_z)] + \alpha T + \epsilon_{rc}$$

$$\epsilon_\theta = \frac{1}{E} [\sigma_\theta - \nu (\sigma_r + \sigma_z)] + \alpha T + \epsilon_{\theta c}$$

$$\epsilon_z = \frac{1}{E} [\sigma_z - \nu (\sigma_r + \sigma_\theta)] + \alpha T + \epsilon_{zc} \quad \dots (3)$$

where σ and ϵ denote the stresses and strains and the suffixes r, θ and z denote radial, circumferential and axial directions. Suffixes, r_c, θ_c and z_c denote the permanent components, in r, θ and z directions. T is the temperature difference between the hot zero power clad (reference state) and the actual temperature at which calculations are conducted.

The permanent strains are given by :

$$\epsilon_{rc} = \frac{\epsilon_{eqc}}{\sigma_{eq}} [\sigma_r - 0.5 (\sigma_\theta + \sigma_z)]$$

$$\epsilon_{\theta c} = \frac{\epsilon_{eqc}}{\sigma_{eq}} [\sigma_\theta - 0.5 (\sigma_z + \sigma_r)]$$

$$\epsilon_{zc} = \frac{\epsilon_{eqc}}{\sigma_{eq}} [\sigma_z - 0.5 (\sigma_r + \sigma_\theta)] \quad \dots (4)$$

where ϵ_{eqc} is the equivalent permanent strain and σ_{eq} is the equivalent stress.

The equivalent stresses and strains are calculated by using deformation energy theory and are given by ;

$$\sigma_{eq}^2 = 0.5 [(\sigma_r - \sigma_\theta)^2 + (\sigma_\theta - \sigma_z)^2 + (\sigma_r - \sigma_z)^2]$$

$$\epsilon_{eq}^2 = \frac{2}{9} [(\epsilon_r - \epsilon_\theta)^2 + (\epsilon_\theta - \epsilon_z)^2 + (\epsilon_z - \epsilon_r)^2] \quad \dots (5)$$

Again as permanent strains due to creep and time independent plasticity are assumed to occur at constant volume they satisfy the equation

$$\epsilon_{rc} + \epsilon_{\theta c} + \epsilon_{zc} = 0 \quad \dots (6)$$

The time independent plasticity law used in this code is of the type ;

$$\epsilon_p = M \sigma_{eq}^N \quad \dots (7)$$

where ϵ_p is the time independent equivalent plastic strain; M and N are material constants based on (Ref.7).

Creep equation used in this code is based on multimechanism creep model and is dependent on temperature, fast neutron flux ($> 1\text{Mev}$) and stress level (Ref.6).

The final equations for stresses and strains are obtained by using equations (1) to (7) and are as follows:

$$\sigma_r = Y + \frac{E}{1+\nu} (\epsilon_r - \epsilon_{rc})$$

$$\sigma_\theta = Y + \frac{E}{1+\nu} (\epsilon_\theta - \epsilon_{\theta c})$$

$$\sigma_z = Y + \frac{E}{1+\nu} (\epsilon_z - \epsilon_{zc})$$

where $Y = \frac{E}{1-2\nu} \left[\frac{\nu}{1+\nu} (\epsilon_r + \epsilon_\theta + \epsilon_z) - \alpha T \right] \dots (8)$

and $\epsilon_r = G [\alpha T - P] + H \left[\epsilon_{rc} + \frac{R}{2} - \frac{Q}{2} \right] + A_1 - \frac{A_2}{r^2}$

$$\epsilon_\theta = GP + \frac{H}{2} [Q + R] + A_1 + \frac{A_2}{r^2}$$

$$\epsilon_z = A_3$$

where $G = \frac{1+\nu}{1-\nu}$, $H = \frac{1-2\nu}{1-\nu}$

$$P = \frac{1}{r^2} \int_{r_i}^r \alpha T r dr, \quad Q = \frac{1}{r^2} \int_{r_i}^r r (\epsilon_{rc} + \epsilon_{\theta c}) dr$$

$$R = \int_{r_i}^r \frac{\epsilon_{rc} - \epsilon_{\theta c}}{r} dr \dots (9)$$

where r_i is the inner cladding radius. The integration constants A_1 , A_2 , A_3 are determined using the following boundary conditions:

$$(\sigma_r)_{r_0} = -P_{\text{coolant}}, \quad (\sigma_r)_{r_i} = -(P_{\text{gas}} + P_{\text{contact}})$$

and $\int_{r_i}^{r_0} \sigma_z r dr = 0.5 (P_{\text{gas}} r_i^2 - P_{\text{coolant}} r_0^2) + F_{\text{contact}} \dots (10)$

where P denotes pressure, F denotes force and r_0 is the outside cladding radius.

In the absence of physical contact between cladding and fuel pellets P_{contact} and F_{contact} are zero and during interaction these two parameters are determined as follows:

$$P_{\text{contact}} = C_Y (r_{\text{fuel}} - r_{\text{clad}})$$

$$F_{\text{contact}} = C_Z (\epsilon_z^{\text{fuel}} - \epsilon_z^{\text{clad}}) \dots (11)$$

where r_{fuel} and r_{clad} denote the fuel and inner clad radius in the case of unrestricted deformation and ϵ_z^{fuel} and ϵ_z^{clad} are corresponding strains in axial direction. C_Y and C_Z are interaction constants and are dependent on fuel and cladding, temperatures and dimensions at the instant of interaction.

C_Y is calculated by assuming fuel to have a plastic core of the diameter corresponding to the temperature distribution and exposure, and it interacts with a hollow outer tube (cladding). Both fuel and cladding are assumed to undergo

deformation due to fuel clad differential expansion. The following equation is used to calculate C_r and is based on stress-strain relation for a thick cylinder.

$$C_r^{-1} = \frac{r_i}{E_{eqcl}} \left(\frac{r_o^2 + r_i^2}{r_o^2 - r_i^2} + \nu_{eqcl} \right) + \frac{r_{fa}}{E_{eqf}} \left(\frac{r_{fa}^2 + r_p^2}{r_{fa}^2 - r_p^2} - \nu_{eqf} \right) \quad \dots (12)$$

where r_{fa} is the actual fuel radius at that instant. r_p denotes the radius at which elastic zone of fuel begins and is dependent on temperature distribution.

Again E_{eqcl} , E_{eqf} , ν_{eqcl} , ν_{eqf} are the equivalent Young's moduluses and Poissons ratios for clad and fuel, and are evaluated as follows :

$$E_{eqcl} = \frac{\sum_{i=1}^{i=n_c} E_{ci} A_{ci}}{A_c}, \quad E_{eqf} = \frac{\sum_{i=1}^{i=n_{fc}} E_{fi} A_{fi}}{A_f}$$

$$\nu_{eqcl} = \frac{\sum_{i=1}^{i=n_c} \nu_{ci} A_{ci}}{A_c}, \quad \nu_{eqf} = \frac{\sum_{i=1}^{i=n_{fc}} \nu_{fi} A_{fi}}{A_f} \quad \dots (13)$$

where E_{ci} , E_{fi} , ν_{ci} , ν_{fi} are the cladding and fuel young's Modulus and Poissons' ratio corresponding to the average temperature in the particular annulus (cladding or fuel) under consideration. A_{ci} , A_{fi} are the areas of the fuel and cladding annuli where fuel elastic zone is divided into n_{fc} number of annuli and cladding into n_c number. A_c and A_f refer to the total area of cladding and elastic fuel. For C_z calculation also, fuel is assumed to have a plastic core of the diameter corresponding to temperature distribution and both fuel and cladding undergo deformation due to fuel clad differential expansion. C_z is given by the following equation :

$$C_z^{-1} = \left[\frac{1}{E_{eqcl} A_c} + \frac{1}{E_{eqf} A_f} \right] + \frac{3}{\pi} \left[\frac{1}{t_c r_i E_{eqcl}} + \frac{1}{t_f r_{fa} E_{eqf}} \right] \quad \dots (14)$$

where t_c and t_f denote the cladding and fuel elastic zone thickness. The second term in the above equation is due to bending and is important for small diameter fuel pins with thin cladding. Inclusion of the bending term in modelling results in lower value of $F_{contact}$ and may or may not give conservative results depending on the other variables. To account for fast power ramps the material properties are taken from the values corresponding to the beginning of the ramp and dimensions are based on the conditions at the end of the ramp. This approach results in higher values of C_r and C_z .

3.0 Solution of the equations:

The temperatures, stresses, strains etc. are calculated at all the node points of the cladding; temperature distribution is also calculated at all the node points

of the fuel for every point of the input power history. Briefly the step by step calculation procedure adopted in the code is as follows:

- 3.1 From the coolant temperature, heat transfer coefficient and heat flux input the cladding temperature distribution and properties are calculated and are converged by bisection method.
- 3.2 Assuming a fixed value of gap conductance fuel temperature distribution fuel material properties, densification and relocation parameters, fission gas release, gas pressure, gap conductance etc. are calculated and are converged by bisection method.
- 3.3 Cladding and fuel mechanical properties are calculated for each annulus using the average temperature for that annulus.
- 3.4 Equations (12) to (14) are used to calculate interaction constants using the material properties for fuel and cladding based on the average temperature of the annuli.
- 3.5 Contact pressure and contact force are calculated by using assumed value of ϵ_{θ} , ϵ_z and equation (11), which are substituted in equation (10) to get the boundary conditions.
- 3.6 Assuming some values for permanent strains, constants A_1 , A_2 , A_3 in equation (9) are calculated by the solution of linear equations by Gaussian method. The stresses and strains are calculated by equation (8) and (9) which are substituted in equation (5) to find the equivalent stresses and strains.
- 3.7 Equivalent stresses are used in creep and time independent plasticity equations to compute the permanent strains at each node.
- 3.8 The permanent strains, calculated in 3.7, are matched with the assumed values in 3.6. ϵ_{yc} and $\epsilon_{\theta c}$ are converged by Newton Raphson method (Ref.5). In this method convergence is strongly dependent on the values of the partial derivatives of the functions which are calculated by finite difference method. The accuracy of these derivatives depend on the increment of variables. This increment is varied in the code for every iteration to achieve accuracy and convergence.
- 3.9 ϵ_{θ} and ϵ_z are used to calculate contact pressure and contact force and are converged by using the latest values of the contact pressure and force.

4.0 Results and Conclusions:

The input data for two different types of fuel pins operating with same power history; and the stresses and strains in the cladding are given in Table-I, and Table-II.

Experimental verification of the computer code is in progress at pressurized water loop, CIRUS, with natural and mixed oxide fuel pins of different diameters chosen on the basis of test section size and fabrication capability. The irradiation

programme is carried out with two types of clusters; six rod cluster with triangular array for the larger diameter pins and eight rod cluster with square array for smaller diameter pins. At present the code has been commissioned and is being verified by the available irradiation data. In future this code will be modified to accommodate dynamic temperature rise during fast power transients.

Reference :

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Table-I
Input Data

	Clad Material	Clad o.d. (cms)	Clad I.d. (cms)	Fuel Material	Pellet diameter (cms)	Pellet Density	Operating pressure (kg/cm ²)	Mean coolant Temp. (°C)
Case I	Zr-4	0.72	0.6	UO ₂ +PuO ₂	0.593	95%	140	253
Case II	Zr-4	1.43	1.2636	UO ₂ +PuO ₂	1.24	95%	72	286

Table-II
Fuel Pin Operation History and Stresses &
Strains at Clad Inside Surface

Sr. No.	Operat- ion time (hrs)	Heat Flux W/cm ²	Case-I						Case - II					
			ϵ_{vc} $\times 10^{-4}$	ϵ_{ec} $\times 10^{-4}$	ϵ_r $\times 10^{-4}$	ϵ_θ $\times 10^{-4}$	σ_{eq} kg/cm ²	σ_θ kg/cm ²	ϵ_{vc} $\times 10^{-4}$	ϵ_{ec} $\times 10^{-4}$	ϵ_r $\times 10^{-4}$	ϵ_θ $\times 10^{-4}$	σ_{eq} kg/cm ²	σ_θ kg/cm ²
1	0	5.0	0	0	6.84	-7.64	783	-904	0.0	0.0	5.07	-5.51	555	-641
2	0	116.9	0	0	4.66	-6.34	569	-638	0.0	0.0	1.42	-3.58	309	-287
3	250	116.9	.455	-0.6	5.34	-7.03	582	-657	0.098	-0.234	1.66	-3.82	309	-296
4	500	116.9	.94	-1.19	6.01	-7.7	593	-672	0.216	-0.468	1.88	-4.04	307	-303
5	500	5.0	1.09	-1.1	8.16	-9.01	809	-837	0.402	-0.408	5.53	-5.98	561	-651
6	500	128.6	0.928	-1.21	5.75	-7.57	571	-645	0.176	-0.463	1.46	-3.84	291	-268
7	600	116.9	0.951	-1.2	6.01	-7.69	591	-671	0.218	-0.467	1.87	-4.03	306	-302
8	750	116.9	1.45	-1.8	6.67	-8.37	602	-687	.337	-0.7	2.09	-4.25	305	-308
9	1000	116.9	1.97	-2.41	7.33	-9.02	609	-697	.477	-0.932	2.29	-4.45	302	-313
10	1250	116.9	2.51	-3.03	7.98	-9.68	616	-707	.615	-1.15	2.49	-4.64	299	-315
11	1500	116.9	3.07	-3.64	8.63	-10.3	621	-716	.761	-1.38	2.67	-4.83	296	-317
12	1500	90.0	3.17	-3.57	9.19	-10.6	671	-776	.935	-1.35	3.61	-5.28	348	-393
13	1750	90.0	3.68	-4.16	9.75	-11.2	672	-779	1.09	-1.56	3.79	-5.46	345	-398
14	1750	125.0	3.69	-4.15	9.23	-10.5	600	-693	0.844	-1.61	2.54	-4.85	277	-293
15	1750	120.0	3.58	-4.23	9.13	-10.8	615	-709	0.89	-1.61	2.72	-4.94	286	-306
16	2000	120.0	4.15	-4.85	9.78	-11.5	621	-718	1.03	-1.82	2.9	-5.11	282	-308
17	2250	120.0	3.52	-5.8	7.67	-12.7	612	-661	1.17	-2.03	3.06	-5.28	278	-307
18	2500	120.0	2.33	-6.2	3.74	-9.95	342	-372	1.33	-2.24	3.21	-5.42	273	-306
19	2750	120.0	1.58	-6.41	2.71	-10.8	392	-389	1.46	-2.44	3.36	-5.56	268	-303
20	2750	5.0	5.78	-5.82	13.2	-14.1	850	-991	2.11	-2.14	7.14	-7.62	550	-653
21	2750	129.0	5.1	-5.08	10.3	-12.3	595	-692	1.39	-2.45	3.01	-5.4	252	-278