COMETHE III-M FOR TRANSIENT FUEL ROD BEHAVIOUR PREDICTION

M. BILLAUX, J. VAN VLIET
Belgonucléaire,
Brussels,
Belgium

SUMMARY.

The COMETHE III-M version is being developed in order to provide fuel rod behaviour prediction capability both in steady-state and in transient situations. It also allows to estimate the fuel rod enthalpy evolution versus time or burnup which may be important in core-related safety studies.

This paper describes the transient heat transfer models, including transient heat conduction inside the fuel rod, and a subchannel model providing transient flow as well as enthalpy calculation capability. Transient fission gas release is also modelled on basis of the change rate of oxide temperature. The models are illustrated by a few calculation examples.

1. INTRODUCTION.

After COMETHE III-L already presented at this conference [1, 2, 3], COMETHE III-M represents the next step in BELGONUCLEAIRE effort to develop a fuel rod behaviour code providing simultaneous steady-state and transient prediction capability. This twofold capability is necessary because the analysis of some operational and accidental reactor transients has to demonstrate that design margins or regulatory limits are not exceeded. The predictions have to be quantitatively as accurate as reasonably feasible, in order not to unduly restrain fuel utilization or reactor operation.

As one has to consider in most of the transients fuel rods which have been pre-irradiated, it was considered necessary from the beginning to merge in the same fuel rod code models related to steady-state as well as transient rod behaviour.

This policy also allows the evaluation of post-transient or post-incident fuel rod behaviour which presents a direct interest for reactor operator. On the other side, it is required that the same model handles with situations where the time scale ranges from the order of weeks down to the order of seconds or less.

The development of the transient version of COMETHE has been described in previous papers [4, 5]. This paper aims at presenting the main models involved in the transient calculations that can be performed by COMETHE III-L. It also illustrates the model capabilities in a few calculation examples.

2. TRANSIENT HEAT TRANSFER INSIDE THE FUEL ROD.

The transient heat transfer is calculated in COMETHE III-M by solving the one-dimensional radial heat conduction equation, with as outer boundary condition a convection relation :

$$k_c \left.\frac{\partial T}{\partial r}\right/_{cs} = h_f \left[T_{cs} - T_f(t) \right]$$

where k_c is the clad conductivity, T_{cs} is the clad surface temperature, and h and T_f are respectively the film heat transfer coefficient and coolant temperature estimated on basis of a separate calculation described in next section.

Transient temperatures are calculated using a variational procedure described in [4], i.e. the Lebon-Lambermont restricted variational principle [12]. The fuel rod being described by concentric ring, the trial temperature field consists of finite elements, i.e. piecewise polynoms of the fourth degree, determined on basis of ring boundaries temperatures as well as ring volume averaged temperatures. The extremum condition for the variational principle provides then a system of linear ordinary differential equations which can be integrated on time e.g. by the Euler or Crank-Nicholson implicit schemes, providing for each time step a system of linear equations. The symmetric matrix of this system exhibits the so-called 3 x 3 block diagonal structure, which allows an easy direct inversion.

The coupling with COMETHE of the transient heat conduction algoritm is optimized in order to reduce computer running time :

i) Transient conduction calculations are performed if and only if they are required : this is made possible by monitoring heat balance in the fuel rod together with thermal boundary conditions and power generation rate ;

ii) The COMETHE time step may be different from the transient conduction time step which is selected on basis of numerical stability and accuracy. Conduction time steps as large as 10 to 20 % of pellet thermal time constant, i.e. time steps of the order of 1 second are possible : this means that in most transient calculations cases there will be one transient heat conduction time step for one COMETHE time step.

Other features of the fuel rod heat transfer model are fuel melting calculation and the possibility to represent steep temperature gradients :

i) Fuel melting and the corresponding melting latent heat and fuel expansion are treated in COMETHE III-M, from the thermal as well as mechanical standpoint. However, effect of fission gas upon melting and molten fuel extrusion into cracks is not yet considered ;

ii) The use of piecewise polynoms of the fourth degree in the radial coordinate allows a good accuracy of the calculated temperature field, even in the peripheral zone of the fuel pellet where finite differences usually provide a poor result ; the requirement for the gradient accuracy originates from the fact that the latter gradient may be responsible of fuel fragmentation and transient gas release, as described in Section 4.

3. TRANSIENT BEHAVIOUR OF THE COOLANT.

When the variations of the inlet pressure or of the power transferred to the coolant become significant in time periods shorter than one second the steady state equations of the thermohydraulics are less and less valid. It becomes necessary to generalize the formalism and to introduce transient notions like the inertia and the heat capacity of the coolant.

As in steady state situation the fluid has to obey the three basic conservation laws : the laws of conservation of mass, momentum and energy. But this time the equations derived from these laws contain partial derivatives which make their resolution more difficult. These equations are written here in one dimensional geometry and in eulerian coordinates as they have been programmed in COMETHE III-M :

- Continuity equation :

$$\frac{\partial(\rho v)}{\partial z} = 0$$

- Momentum equation :

$$\frac{\partial (\rho v)}{\rho t} + \frac{\partial}{\partial z} (\rho v^2) = - \frac{\partial p}{\partial z} - \frac{\lambda}{D} \cdot \frac{\rho / v / v}{2} - g \rho$$

- Energy equation :

$$\rho \frac{\partial H}{\partial t} + \rho v \frac{\partial H}{\partial z} = \frac{P_c}{A} h_f (T_{cs} - T_r) + \frac{P_s}{A} h_s (T_s - T_r) + S$$

where ρ is the coolant density, v the velocity, λ the friction factor, D the hydraulic diameter of the channel, g the gravity constant, H the enthalpy, P_c the wetted perimeter of the clad, P_s the wetted perimeter of the structure, A the surface of the channel, T_s the temperature of the structure, h_s the heat transfer coefficient between coolant and structure and S the heat source in the coolant. T_{cs} , the clad surface temperature is known from the thermal calculation of the fuel rod presented above.

The momentum equation is integrated along the whole coolant channel, which allows to calculate the transient coolant flow rate from the transient inlet and outlet pressures. The momentum and the energy equations are solved by a finite difference method. From the first one are derived the pressure distribution in the channel and the saturation temperature at each axial level and from the second one the axial temperature distribution and the margin to boiling.

This models allows to calculate a square, triangular or annular single channel of a fuel element with grids or wire wraps, or of a test loop. The foot, the head and the flow regulating orifice of the fuel element or of the loop are simulated in such a manner that the programme could easily be linked to a code describing the primary circuit of a reactor. The thermal inertia of the structures is described, which is of particular interest for the interpretation of experiments carried out in test loops.

The model is able to consider deformed geometries such as the ballooning of the fuel rods. The reversal of the coolant flow is allowed, which is essential for some safety studies. The two-phase flow has not been implemented in COMETHE III-M. A simple homogeneous model is in preparation and will be introduced in a subsequent version of the programme.

Fig. 1 illustrates a flow reversal resulting from a loss of pressure at the inlet of a channel.

4. TRANSIENT GAS RELEASE.

It has been observed that most of the fission gas is released during fuel temperature transients such as power increases or shut downs [6]. Moreover, transient nuclear heating of pre-irradiated oxide samples has shown increasing gas release with increasing heating rates [7]. A similar trend was exhibited by similar investigations pertaining to DEH tests on preirradiated PWR fuel [8]. This may be interpreted in terms of fuel fragmentation under the effect of very rapid oxide temperature variations, like those obtained by quenching of a rod operated under film-boiling conditions [9]. This fragmentation can be explained in terms of grain boundary fracture mechanics [10], taking into account the ductility induced by grain boundary diffusion.

Oxide fragmentation may occur only all locations in the oxide, leading to total grains separation, i.e. fuel powdering [9]. Grain separation may also be not complete, resulting in fragmentation in larger pieces, i.e. "chunk" break-up [11], inducing however the loss of pellet integrity. These processes lead, as observed in [8] to a significant increase in fuel specific surface. Moreover, the transient gas release may be correlated to the fragmentation induced new pore-solid surface [8]. The latter forms the basis for the transient gas release model presented here, which is already implemented in COMETHE III-L.

The first important element described in this model is the reference temperature T_r corresponding to the temperature where the intergranular fission gas bubbles could be in hydrostatic equilibrium. This equilibrium is due to redistribution of UO around the existing porosities or cracks, mainly by surface or grain boundary diffusion. If θ is the time, T the actual oxide temperature and τ a time constant, the considered relation is :

$$\frac{dT_r}{d\theta} = -\frac{1}{\tau}(T_r - T)$$

The transient gas release calculation is based on a diffusion model based on an equivalent diffusion sphere radius, as described in [1]. The latter radius is defined starting from the actual fuel open porosity ξ. During the transient, the latter quantity is replaced by an effective open porosity ξ_e as defined by the following relation :

$$\frac{d\xi_e}{d\theta} = k(\dot{T})\, v\, \frac{\dot{T}}{T_r} - \frac{\xi_e - \xi}{\tau}$$

In this relation, the first term describes open porosity creation as a result of the temperature increase rate T. The quantity v denotes the fission gas swelling, while k(T) is a temperature rate dependent proportionality constant. The second term describes the progressive intergranular crack healing. In this way, the equivalent sphere out of which fission is diffusing sees its radius transiently decreased to simulate intergranular separation.

This model has been partly verified against the Inter-Ramp data, the corresponding comparison between calculation and measurements is reported in [2]. It has also been applied to LWR fuel rod calculations. As example, the transient gas release from a BWR 8 x 8 fuel rod submitted to a power ramp has been analysed. The rod is made up of fuel pellets presenting a very low open porosity (0.1 %) as it is the case in the modern fabrication lines. It is filled with helium at 1 bar. Two COMETHE calculations have been performed. In the first one the fuel rod is irradiated for 700 days at constant power : 260 W/cm at the power peak in the lower part of the fissile column. In the second one the fuel rod is irradiated for two cycles of 340 days at the same power level. The two cycles are separated by a shut down and a fast restart. This one is simulated by a power ramp of slightly less than 15 minutes (from 30 to 260 W/cm at the power peak). Fig. 2 shows the additional transient gas release resulting from the ramp : it amounts to 8 % in only one day.

5. SAMPLE CALCULATIONS.

In order to illustrate, COMETHE III-M has been applied to simulate two typical LWR power transients.

(a) Control Rod Ejection Accident.

Fig. 3 represents the evolution of a fresh PWR 17 x 17 fuel rod subjected to a power transient representative of the overpower transient resulting from fast rod ejection. The power which is initially very low raises in about 50 msec up to 10000 W/cm. After 100 msec, the power stabilizes at 150 W/cm, for a few seconds, until shut-down. Energy deposition during the transient amounts to 230 J/g UO2.

As shown by Fig. 3, peak temperatures reach quickly more than 1000°C, with as result the mechanical interaction depicted on Fig. 4. Final permanent clad strains are negligible, which is to be attributed to the low deposited energy : one is still far from the typical failure treshold of about 1 kJ/gUO2, for fresh fuel.

(b) BWR Turbine Trip Transient.

Figs. 5 and 6 describe the time evolution of a 8 x 8 unpressurized BWR fuel rod, preconditioned up to 20 GWd/tox at a linear power of 240 W/cm. The power evolution during the transient is provided in Fig. 5.

The thermal effect of the transient is not important as peak temperatures raise only by about 110°C. However, as the rod underwent overheating during steady-state, the gap at ridge location is practically closed, the temperatures are high and FGR amounts to 16 %. This results in a hoop stress pulse of about 120 MPa, which is quickly relaxed.

CONCLUSION.

This paper has presented the main features of the COMETHE III-M fuel rod behaviour code, for steady-state as well as transient prediction. The different models capabilities have been illustrated by a few representative examples, such as flow reversal, transient gas release and typical PWR and BWR transients. Adequate coupling between thermal and mechanical models, already exhibited for steady-state rod behaviour is now extended to transient calculations.

REFERENCES.

[1] Oxide Behaviour Modelling Progress in COMETHE.
J. van Vliet & N. Hoppe
Presented at this Conference.

[2] Comparison with Experiment of COMETHE III-L Fuel Rod Behaviour Predictions.
J. van Vliet & M. Billaux
Presented at this Conference.

[3] Parametric Study with COMETHE.
M. Billaux & H. Heckermann
Presented at this Conference.

[4] A COMETHE Version with Transient Capability.
J. van Vliet & al.
IAEA-SM on Fuel Element Performance Computer Modelling, Blackpool (March 1978).

[5] COMETHE III-L - A Modified Version to Account for LWR Fuel Behaviour during Ramps and Transient Operation.
N. Hoppe & J. van Vliet
ANS/ENS Topical Meeting on Reactor Safety Aspects of Fuel Behaviour, Sun Valley (August 1981).

[6] Effect of Power Changes on Fission Product Gas Release from UO2 Fuel.
R. Soulhier & M.J.F. Notley
Nucl. Applic. 5 (1968) 296

[7] Transient Fission Gas Behaviour Studies on Irradiated Mixed Oxide in Silene.
M. Cranga & al. - Paper IX/3.
ANS/ENS Topical Meeting on Reactor Safety Aspects of Fuel Behaviour, Sun Valley (August 1981).

[8] The Mechanistic Prediction of Transient Fission Gas Release from LWR Fuel.
J. Rest & S.M. Gehl
Nucl. Eng. & Design 56 (1980) 233-256.

[9] **Intergranular Fracture of Unrestructured UO2 Fuel during Film-Boiling Operation.**
A.W. Cronenberg & T.R. Yackle
J. Nucl. Mat. 84 (1979) 295-318.

[10] **The Effects of Grain Boundary Fission Gas on Transient Fuel Behaviour.**
R.J. Dimelfi & L.W. Dietrich
Nucl. Tech. 43 (1979) 328-337.

[11] **In-Pile Experimente zum Brennstabverhalten beim Kühlmittelverluststörfall,**
L. Sepold & al.
KfK 30099 (Juli 1981).

[12] G. Lebon & J. Lambermont
Ann. Phys. 32 (1974) 425.

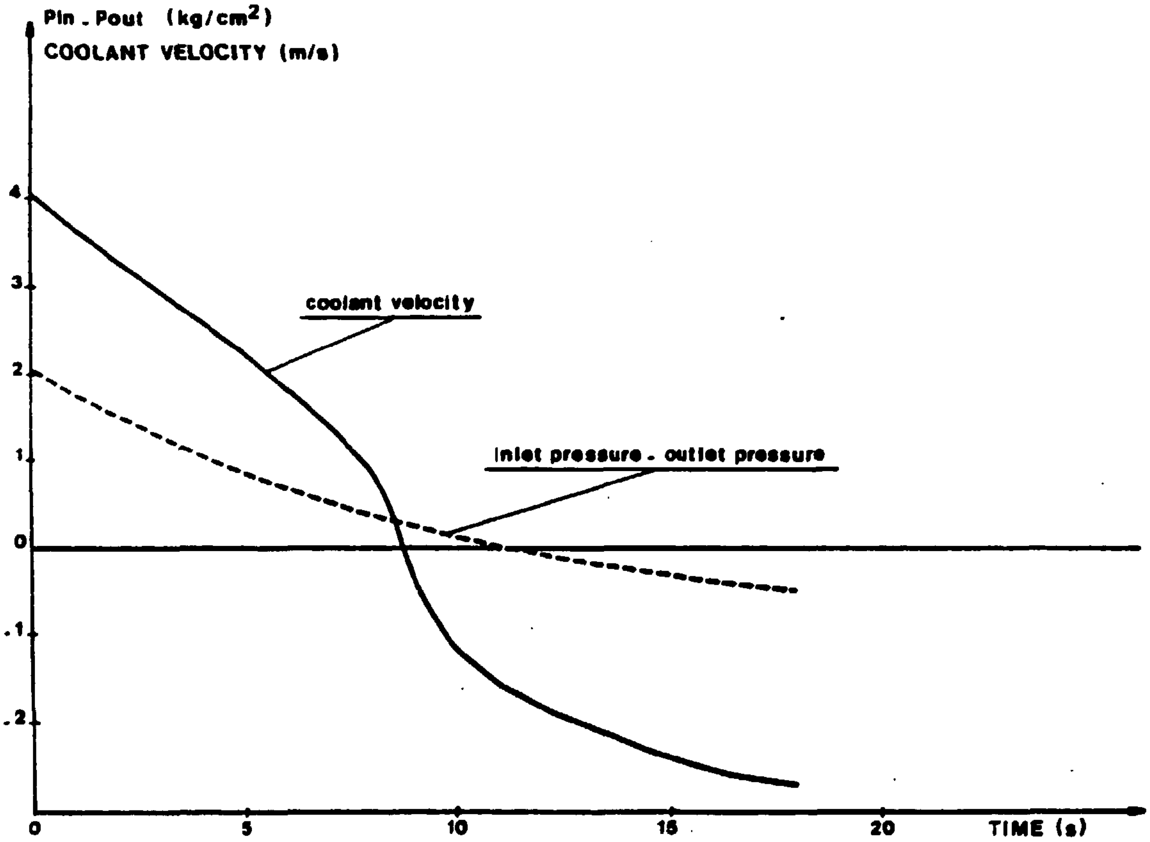


FIGURE 1

TRANSIENT FLOW RATE WITH FLOW REVERSAL

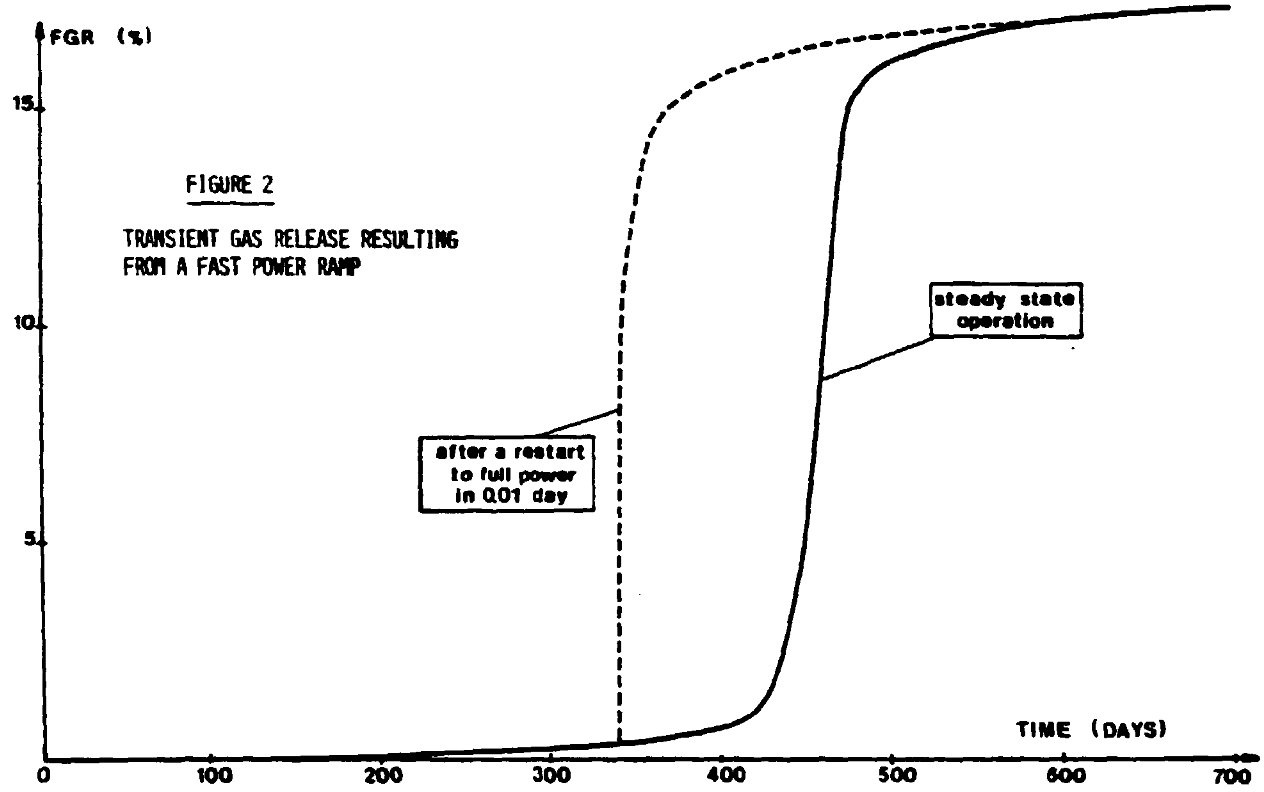
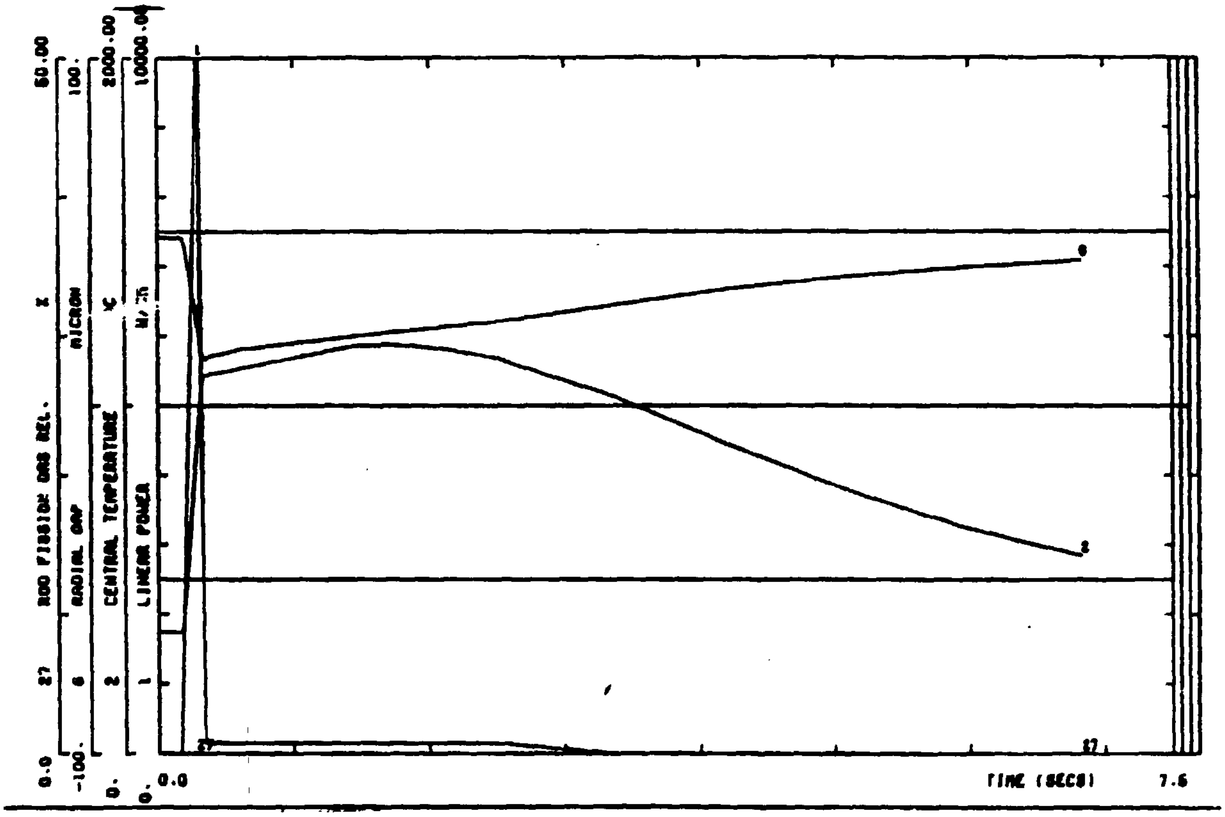


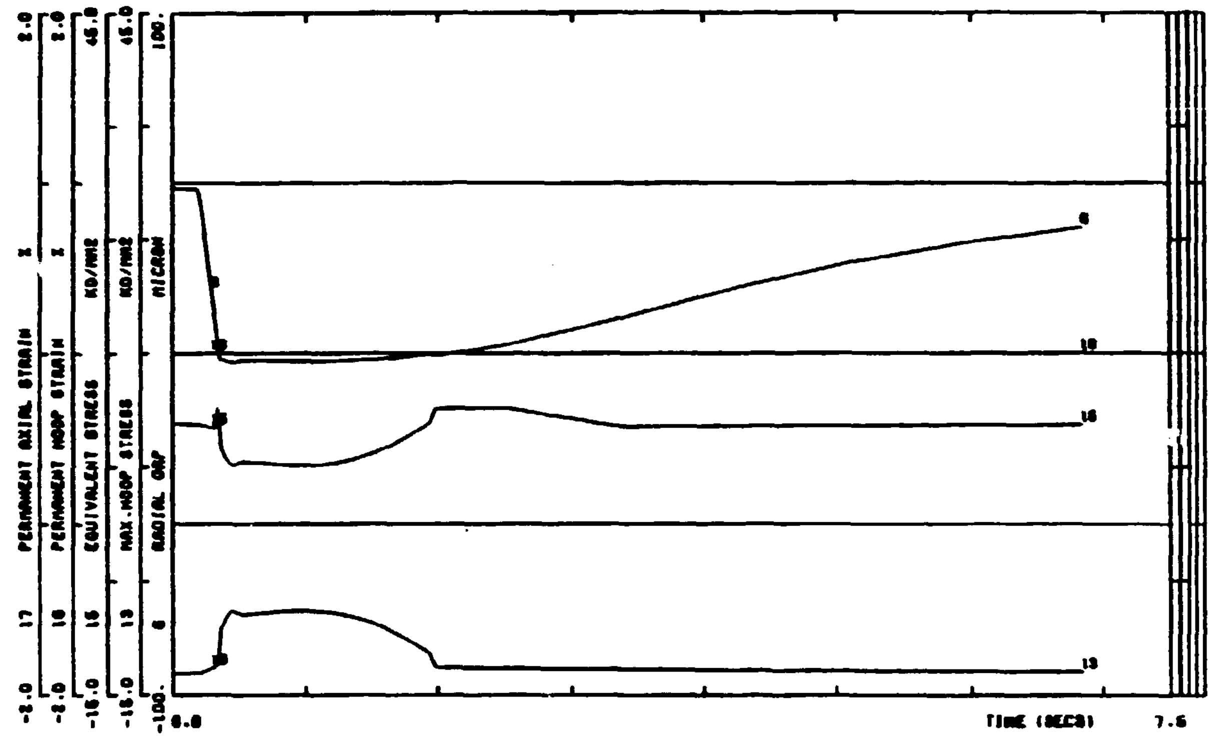
FIGURE 2

TRANSIENT GAS RELEASE RESULTING
FROM A FAST POWER RAMP



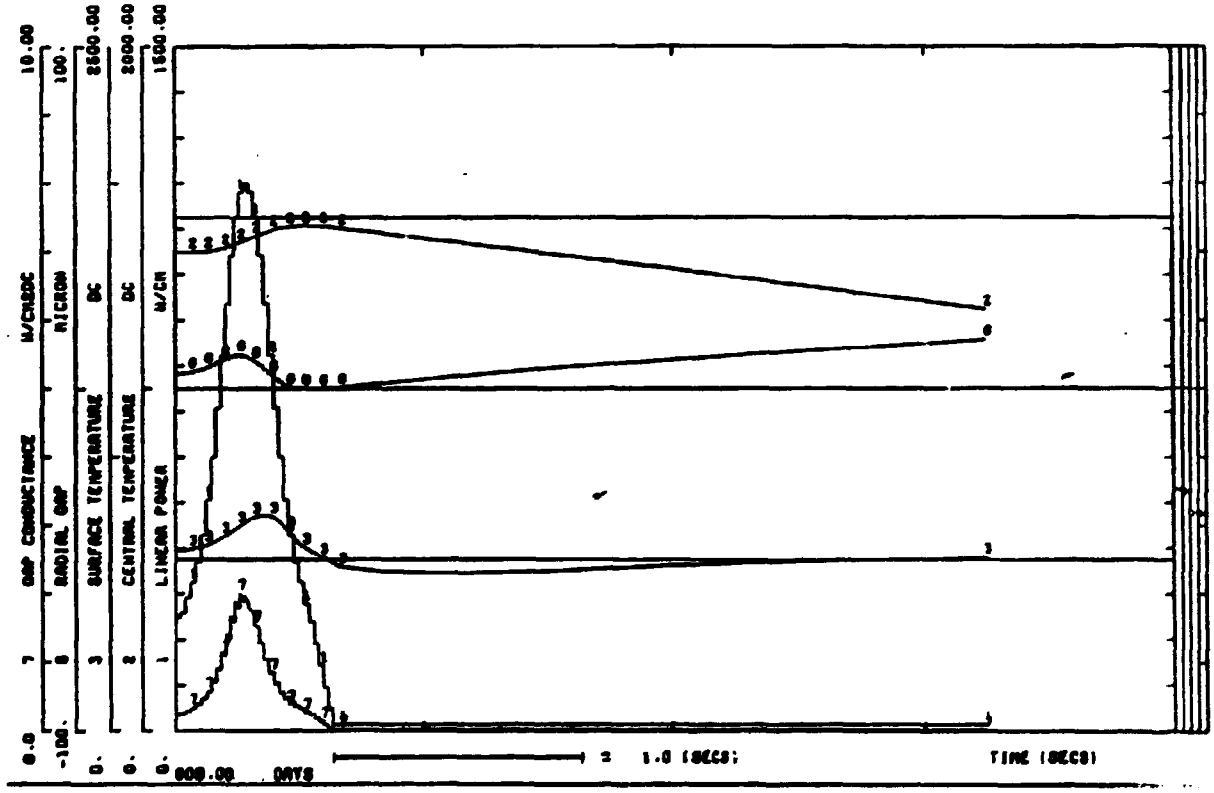
COMETHE IIIMPWR 17X17 ROD EJECTION ACCIDENT
SLICE 1
MID PELLET RESULTS

FIGURE 3



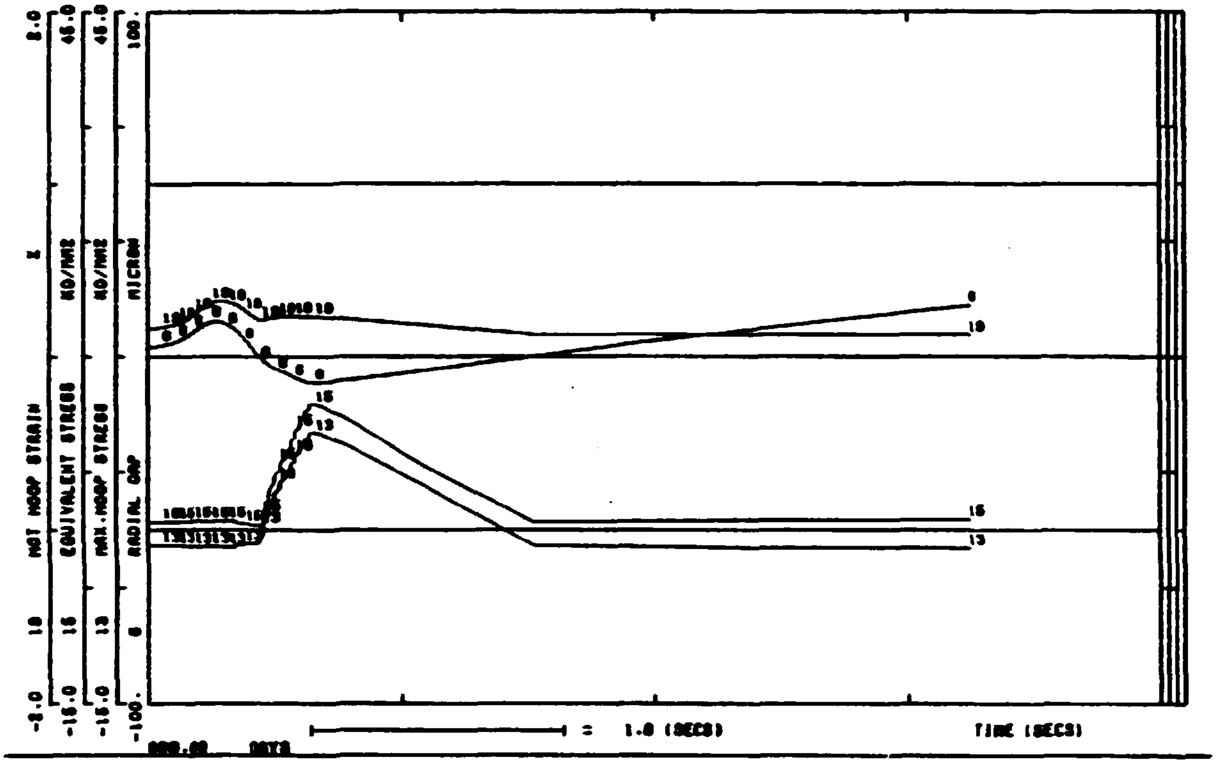
COMETHE IIIM PWR 17X17 ROD EJECTION ACCIDENT
SLICE 2
RIBBING RESULTS

FIGURE 4



COMETHE IIIM BWR FUEL ROD BEHAVIOUR DURING TURBINE TRIP 20000 MWD/T
SLICE 1
RIB PELLET RESULTS

FIGURE 5



CONETHE (III) BWR FUEL AND BEHAVIOUR DURING TURBINE TRIP 23000 MWD/T
SLICE 2
PELLET END RESULTS

FIGURE 6