A METHOD FOR THE NUMERICAL CALCULATION OF THE BEHAVIOUR OF FUEL ELEMENTS

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SUMMARY

The production of viable theoretical model for the complex thermo-mechanical interactions in a fuel element is very desirable in the light of the difficulty and expense involved in performing in-pile experiments. In particular a knowledge of the life-history of such a system is vital for estimates of pin endurance and failure mechanisms.

This work is concerned with the production of such a model which is sufficiently accurate to allow realistic predictions to be made within the physical model adopted whilst being sufficiently economical in computing time to allow full life history analysis of the fuel pin. The problem is divided into two distinct, though related parts: firstly the empirical parameterization of the material properties such as creep, swelling and the thermal properties and secondly the purely mathematical problem of the solution of the resulting equations. It is on this second part that we have concentrated our effort to produce a computer programme which is sufficiently accurate and flexible to accommodate any particular parameterization which may be required. Existing methods are based on inadequate numerical procedures which may lead to inaccuracies and instabilities. The present method avoids these difficulties by means of sophisticated matrix handling techniques which are extremely rapid and allow a detailed description of the system by the economic use of fine spacial and time steps. No iterative procedures are involved and there are therefore no difficulties in making first predictions, inaccuracies in which can lead to instability. The system of equations is linearized and then solved exactly by a specially developed technique. The errors involved in the linearization are of the same order, or smaller, than those inherent in the numerical approximations.

Extensive testing of the method using a typical model parameterization has been carried out and the method has proved very accurate and reliable. It has been shown to be capable of revealing fine details and cases can be found where less sophisticated methods would be unable to give a realistic description of the behaviour of the system.

Introduction

The design of reactor fuel elements requires knowledge of their behaviour during in-pile operation. Such information is extremely difficult to obtain experimentally and consequently it is desirable to have a physical model of the system which will allow the calculation of the stress-strain history of a fuel element. Such a model has been developed and implemented in the computer programme FRUMP. Important physical effects such as thermal and irradiation creep and irradiation induced swelling have been included in the model. The programme has been constructed to allow the parameterization of these quantities to be altered easily, facilitating, for example, investigation of different empirical and semi-empirical formulae for fuel swelling and irradiation creep.

An important application of such a model is the study of the effects of power cycling the reactor to isolate any possible damaging power changes. Further, fast transients in the power are also very important for studying possible failure situations and the model has been developed so that these may be investigated with good accuracy.

The calculations reported here are a first approximation since the model is still undergoing active development. As a test case we have calculated the stress strain history for a UO_2 fuelled element for just one power cycle. Here we have concentrated on the fuel, although our eventual objective is to give a viable description of the behaviour of the clad.

The system with which we shall be dealing is shown schematically in figure 1. It consists of a pair of axially symmetric cylinders, the inner of which represents the fuel, the outer the cladding material. Figure 1 represents the system before introduction into the reactor, with a fabricated central hole and, in this case a gap between the fuel and clad. The method has been designed to predict the following quantities: the non-linear temperature distribution across the fuel and can, the changes in the dimensions of the fuel and can; the stress distribution in the three principal directions, including a partitioning into thermo-elastic, thermal and irradiation induced creep and deformations by swelling in the fuel and can.

Method of Calculation

The calculation of the stresses and strains in a fuel pin involves the solution of a set of coupled differential equation which describe the balance of stresses within the system and the rate of plastic deformation as a function of time. The stresses are initially caused by the thermal expansion of the material and the temperature distribution will be a function of the strains at any particular time. The time dependence of the basic quantities thus appears in the equation describing the diffusion of heat through the fuel and cladding material, and also in the equations describing the creep and swelling rates. The first versions of the programme neglect the explicit time dependence of the diffusion equation and assume that the temperature is always in a steady state condition. This assumption, which will be relaxed in later versions of the computer programme, restricts the validity of the results to non accident conditions. The creep equations are however treated in the complete time dependent form and since the possibility of high stresses can introduce difficulties of stability, it is desirable to obtain a method which has a high inherent stability. Further methods which rely on extrapolating the stresses and strains from previous times must use carefully devised iteration techniques to converge onto the correct result. The present method avoids these

Also required for the calculation of the temperature distribution is a representation of the fuel-clad interface resistance. When the fuel and clad are in contact we have assumed a thermal resistance of $0.5 \times 10^{-4} kW^{-1} m^2$. The thermal resistance of an open gap is calculated from $(0.5 \times 10^{-4} + 5x \text{ gap width}) kW^{-1} m^2$.

All these quantities have been obtained empirically and are liable to inaccuracies. This is especially true of the open gap thermal resistance and for this reason the programme has been constructed to enable these equations to be altered very simply.

2. Creep rates

The fuel irradiation creep rate is taken as

$$\gamma(day^{-1}) = 6.6 \times 10^{-8} \times \text{Rating } (Wg^{-1}) \ \sigma(MNm^{-2})$$

The fuel thermal creep rate is given by

$$\gamma(day^{-1}) = 6.0 \times 10^{10} \ \sigma(MNm^2) \ \exp(-90 \times 10^3/RT).$$

We have assumed that there is no clad irradiation creep under these conditions and that the clad thermal creep rate is given by

$$\gamma(day^{-1}) = 2.0 \times 10^8 \ \sigma^4(MNm^{-2}) \ \exp(80 \times 10^3/RT)$$

3. Swelling rates

At present, for oxide fuel, the volume swelling rate in the fuel is given by

$$S(day^{-1}) = \text{Rating } (Wg^{-1}) \ (1.2 \times 10^{-7} + \frac{\{1.08 \times 10^{-6} + 0.73 \ S \ B^{-1}\}}{\{1 + \exp(-40S - 4.8)\}})$$

where $S = 3.24 \times 10^{-8} \times B^{0.75} T^{1.5} \exp(-15 \times 10^3/RT)$

and B = Rating (Wg^{-1}) x time (days).

The equivalent expression for carbide fuel is

$$S(day^{-1}) = \text{Rating } (Wg^{-1}) \times 1.36 \times 10^7 \ \{1.26 \times 10^{-13} + (2B \times 10^{-5})^{\frac{1}{2}} \times (1.38 \times 10^{-16} xT - 2.43 \times 10^{-19} \times T^2 + 1.35 \times 10^{-22} \times T^3)\}$$

Clad swelling is only assumed to occur during times when the rating is constant and the total clad swelling is then given by

$$S = 2 \times 10^2 \ \text{time}^{1.5}(\text{days}) \times \exp(-30 \times 10^3/RT)$$

Further data requirements, such as pin dimensions, coolant temperature, rating profiles and materials properties may be chosen for the particular calculations.

Results

As a test case, we have performed calculations on an oxide fuel element, following its stress/strain history through one power cycle. The dimensions of the pin were chosen to be; fuel inner and outer radii 1.1mm and 2.5mm respectively and the equivalent dimensions for the clad were 2.505mm and 2.85mm. These dimensions ensure that the initial gap of 0.005mm will close sometime during the power cycle. The parameters for the power cycle were a linear increase in power from 0 to 250 (Wg^{-1}) in 2 hours, followed by 50 days at this rating, after which the power was reduced from 250 (Wg^{-1}) to 0, again in two hours.

problems by using a matrix technique which solves for all variables simultaneously and thus avoids the necessity of iterating the results. The aim has been to produce a method, applicable to a comprehensive range of fuel element-designs which will enable the calculation to be performed with a high degree of accuracy with the minimum of limitations.

The basic approximation of the method is to linearize the equation describing the plastic flow rate,

$$\dot{\gamma}_p = P_p + F_p(\sigma_r, \sigma_\theta, \sigma_z). \tag{1}$$

The general form used in this equation, where the plastic strain in the direction p, namely γ_p, are related to the functions P and F. It is assumed that

$$\sum_p F_p = 0 \tag{2}$$

so that P would normally be chosen to describe the swelling and F is the stress dependent creep rate. Eq. (1) may be linearized by making a Taylor expansion about the point $(\sigma_r^o, \sigma_\theta^o, \sigma_z^o)$,

$$F_p(\sigma_r,\sigma_\theta,\sigma_z) = F_p(\sigma_r^o,\sigma_\theta^o,\sigma_z^o) + (\sigma_r - \sigma_r^o) \frac{\partial F}{\partial \sigma_r}\Big|_{\sigma_o} + (\sigma_\theta - \sigma_\theta^o) \frac{\partial F}{\partial \sigma_\theta}\Big|_{\sigma_o} + (\sigma_z - \sigma_z^o) \frac{\partial F}{\partial \sigma_z}\Big|_{\sigma_o}. \tag{3}$$

Eq. (3) is then solved exactly, together with the stress equilibrium equation, using the plain strain approximation, appropriate for long cylinders. A method of finite differences is used and the resulting matrix equation is solved using a routine which has been specially written to take advantage of the special form of the matrix which is generated.

The method has proved to be extremely stable even when temperatures well above the fuel melting temperature have been artificially introduced. The errors introduced by the Taylor series expansion become smaller as finer time steps are used, and for typical choices of step length are smaller than or comparable to the errors inherent in the numerical methods. It is easily possible to perform calculations with errors of a few percent with a computing time of a minute or two. The length of time step required depends upon the stresses involved, and a special routine is incorporated in the programme to automatically change the length as conditions vary.

Problem Parameterization

In order to utilize the numerical procedures outlined in the previous section we must first define the quantities which were left as general functions (J.Hedger [1]).

1. Temperature distribution

The temperature distribution across the fuel/can system is calculated according to the following expressions.

Fuel thermal conductivity $= \frac{1}{AF + BFT} + CFT^3$

for oxide fuel and AF + BFT for carbide fuel.

The coefficients are AF=10.042, BF=2.71x10^{-4} and CF=69.0x10^{-12} for oxide and AF=9.5, BF = 4.1x10^{-3} for carbide fuel. The clad conductivity is calculated from AC+BCT, with AC=20.0 and B=0. The units of thermal conductivity are $Wm^{-1}K^{-1}$ and T is the temperature in K.

Extensive tests were made in order to ascertain the optimum operating parameters in terms of radial mesh size and length of time steps. It was found that a radial mesh having 49 points in the fuel and 9 in the clad provided ample accuracy for these test calculations. These points are arranged on a non-linear grid so as to give greater accuracy towards the boundaries. The programme is capable of running with either manual choice of time steps, or, automatically by reference to the error criteria outlined earlier.

a. Fuel behaviour. The amount of data emanating from these calculations is formidable, consequently we shall present the results mainly in graphical form. In Figs. 2 and 3 we show the distribution of the radial, $\sigma(r)$, and angular $\sigma(\theta)$ stress in the fuel for various times during the initial uprating of power and for a short time into the constant rating period. At early times $\sigma(r)$ grows almost symmetrically with respect to r until a maximum compressive stress of approximately - 125 MN/m^2 is reached after 0.05 days, just beyond the mid point of the up ramp. After this time the maximum value falls and is displaced outwards as the stress in the inner regions is relieved through plastic flow due to the increasing temperature. This process continues until, at the end of the up ramp the maximum value of $\sigma(r)$ has fallen to - 25 MN/m^2 and is located approximately 15%R from the outer edge of the fuel. The stress in the inner regions has been reduced to very small values right up to the mid point. Continuing in time onto the constant rating period shows that this process eventually reduces the stress to very small values, typically of the order $10^{-3} MN/m^2$, over the whole of the fuel. In figure 3 we show the equivalent results for $\sigma(\theta)$. In this case, the stress distribution at early times changes from a high compressive stress in the inner regions of the fuel to a tensile stress towards the outer edge. Again with increasing time the innermost stresses are relieved by plastic flow, with the maximum compressive component moving outwards through the fuel. In contrast to the radial stress, $\sigma(\theta)$ only dies away relatively slowly during the constant rating period, becoming very small only after two days. Equvalent values of $\sigma(z)$ have not been plotted since they are very similar to those for $\sigma(\theta)$. The axial variations have been excluded by the assumption of the plane strain approximation. Therefore end effects have not been included in the model.

With the initial conditions chosen for these calculations the gap between the fuel and the clad was found to close after 14.0 ± 0.5 days. The variation of the gap width with time during the constant rating section for various radial mesh sizes is shown in figure 4. The early rapid rise, due to continued thermal expansion of the can, before fuel swelling has become important soon becomes a rather smooth, virtually linear decrease towards closure. The accuracy with which we can calculate the absolute closure time is limited by the fact that we are working in terms of differences in the displacements and that we use a rather simple method of linear extrapolation for predicting the closure time between time intervals. The first of these points is illustrated in figure 5 where we show the variation in TGAP (time to gap closure) with the number of radial mesh points (clad + fuel). Below approximately 50 total points TGAP becomes very badly defined whilst above 50 it rapidly approaches an asympototic value of $\sim$ 14 days.

After gap closure the quantity of interest is the contact pressure between the fuel and the clad. This is shown in figure 6, again for various radial mesh sizes. It rises rapidly after closure to a maximum value of ~ 1.6 MN/m^2, thereafter slowly falling until, after 50 days it reaches a value of ~ 102 MN/m^2. If the calculations are extended in time beyond

50 days at constant rating the gap is found to re-open after some 500 days.

The behaviour of the fuel during reductions in power is summarized in figures 7 and 8. In figure 7 we show the radial stress for various times during the 2 hour down ramp. In this case the stresses are all tensile and, since we have no representation of cracking the values are allowed to reach unacceptably high values. For the case of the hoop stress we have a reversal of the behaviour found for the up ramp in that the outer parts of the fuel are under compression and the inner under tension, showing that cracking will occur in the inner regions.

In this paper we have concentrated on the development of the first phase of the model which was concerned primarily with fuel behaviour. This is necessary since the stresses in the clad and ultimately clad failure can be attributed to its interaction with the fuel.

In order to indicate that the model is capable of investigating fine details of the fuel or clad behaviour we show in figure 9 the variation of gap width during the up ramp for various radial mesh sizes. The most obvious feature is the minimum in the gap width at approximately 1.4 hours. The cause of this minimum lies with the particular choice of parameters for this case, and may be seen to be due to the differential thermal gradient causing the fuel to expand more quickly than the clad initially. However as soon as creep begins to relieve the stress in the inner region of the fuel, the larger coefficient of expansion of the clad will carry it away from the fuel. Eventually, of course, swelling in the fuel will reverse this process, leading to gap closure.

The most accurate value for the minimum gap width is 3.6×10^{-6}m, calculated with a total of 154 points in the radial mesh. Using smaller numbers of mesh points decreases the value of the minimum width without appreciably altering its position in time. In fact premature gap closure is obtained with a 33 point radial grid at 1.3 hours, with subsequent re-opening at 1.5 hours. Calculations with coarser time intervals also caused a premature gap opening. It is interesting to note that even with the coarsest radial mesh the gap width at the end of the up ramp is reasonably well represented, indicating that the premature gap closure has, in this case, had no irreversible effect. It would, however, be possible to chose initial parameters such that errors introduced by such a process could be important when attempting to describe a history of power cycling. Consequently we feel that any model should at least be capable of running at high accuracy to investigate detailed effects, even though this facility may not be called upon for normal fuel pin operating conditions. Since it is the purpose of such a model to isolate pathalogical situations for the system such capabilities are vital.

Computing Demands

Any mathematical model which is to be useful in analysing the behaviour of a fuel pin throughout its life must be both accurate and be economical in terms of its computing requirements. The programme was developed and run on the IBM 370/165 machine at Harwell and in its current form requires 240K bytes storage. This size is flexible in that larger numbers of mesh points would increase this value. With the finite difference method written in the special form outlined earlier, the variation of machine time with number of mesh points is linear, as shown in figure 10. For example, an accurate calculation may be performed with a

total of 106 radial mesh points. When allowing the programme to calculate the optimal time a total of ~ 400 steps were needed, with a time/step of 135 msec, giving a total machine time of approximately 54 seconds. Less accurate calculations may be made with considerable saving in time.

Conclusions

We have shown that, within the restrictions of the model adopted, the method is capable of giving quantitative results for the quantities involved in the interaction between the fuel and the clad in a fuel element operating under fast reactor conditions. The accuracy of the results may be chosen by the user to fit the particular needs of the problem in hand, and can be made very high with only moderate demands in computer time. This facilitates the use of the programme to follow the behaviour of the fuel element through a complicated series of power cycles, approaching the conditions which would be met in an operational reactor. Although the quantities of interest from an engineering point of view are entirely concerned with the clad, i.e. dimension changes and possible failure mechanisms, we have concentrated our attention here on the more difficult problem of the fuel. Various developments to the model are currently being investigated. In particular the effects of fuel cracking are of importance since they have a considerable effect in reducing clad stresses.

[1] Hedger, J., Private Communications.

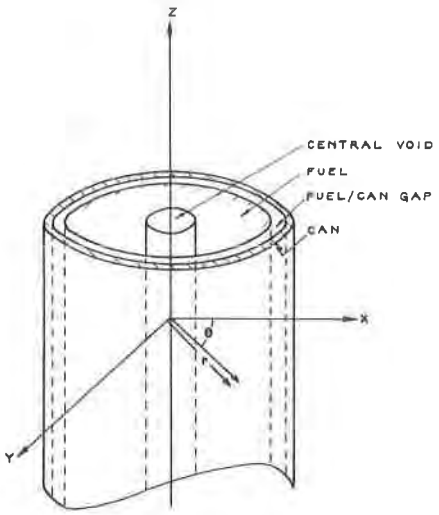


Figure 1 Schematic view of the fuel element before introduction into the reactor.

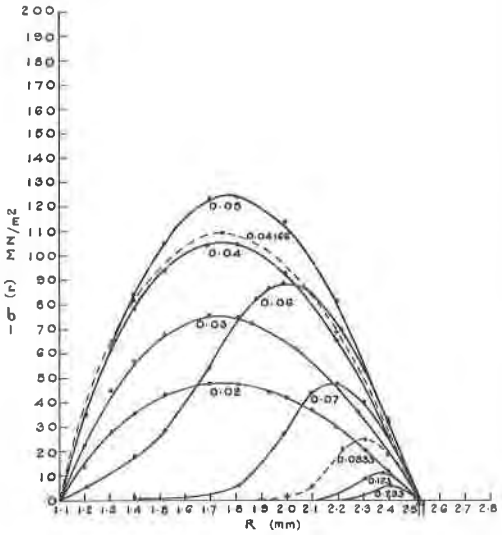


Figure 2 $\sigma(r)$ in the fuel for various times during the up ramp.

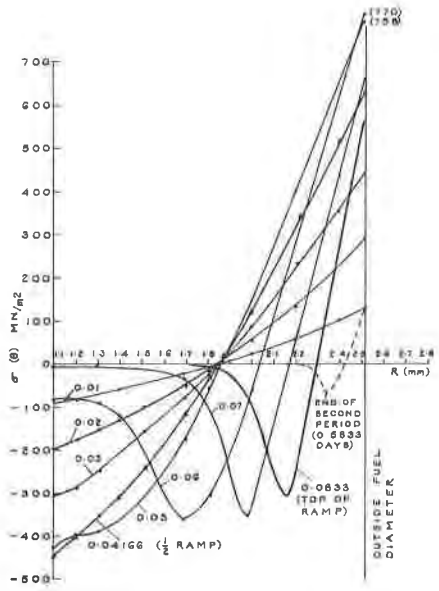


Figure 3 $\sigma(\theta)$ in the fuel for various times during the up ramp.

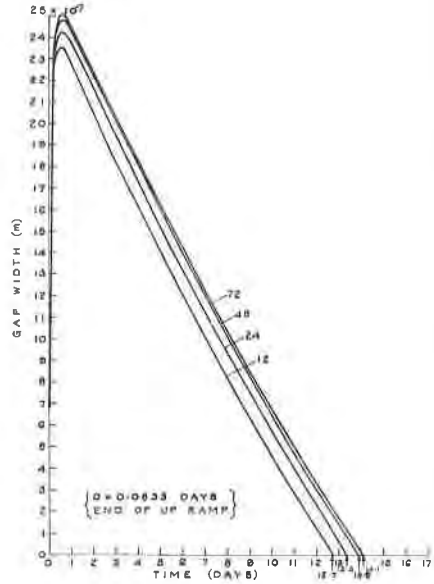
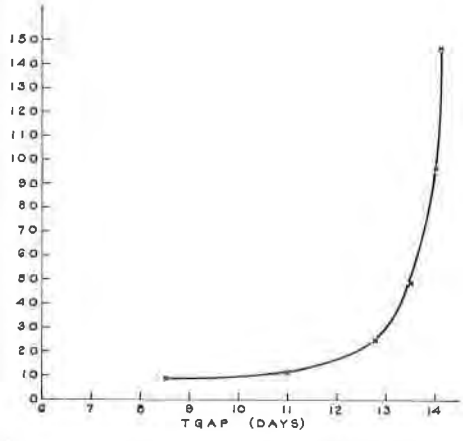


Figure 4 Gap width during constant rating for various radial grid sizes.



gure 5 TGAP as a function of the number radial mesh points.

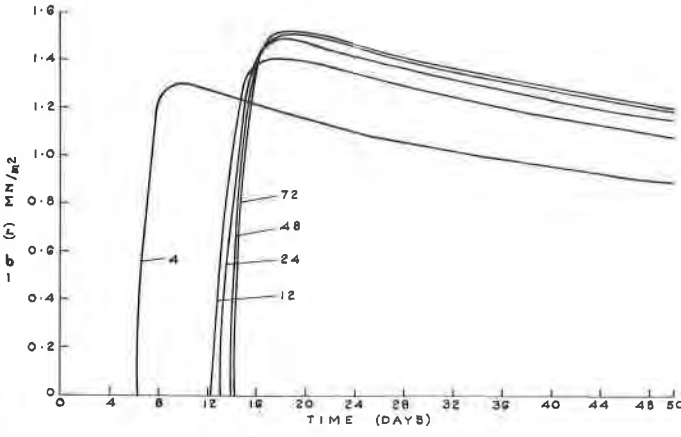


Figure 6 Contact pressure for various mesh sizes.

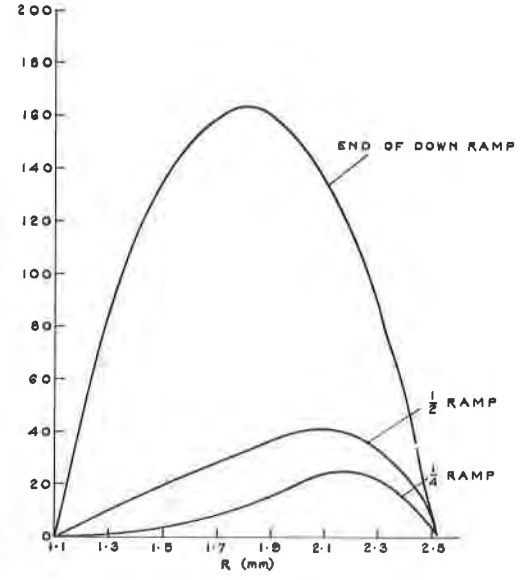


Figure 7 Values of $\sigma(r)$ in the fuel on the down ramp.

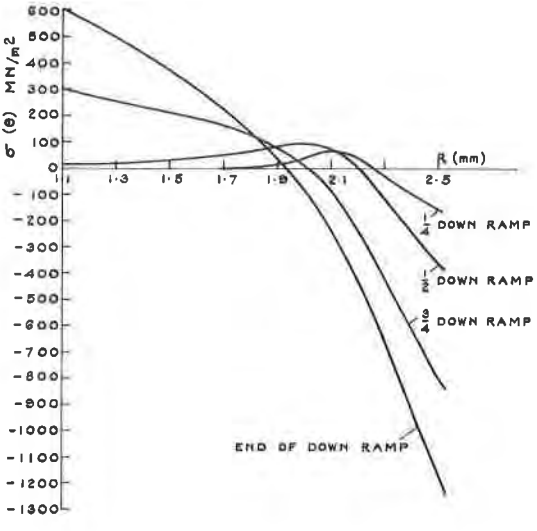


Figure 8
Values of $\sigma(\theta)$ in the fuel on the down ramp.

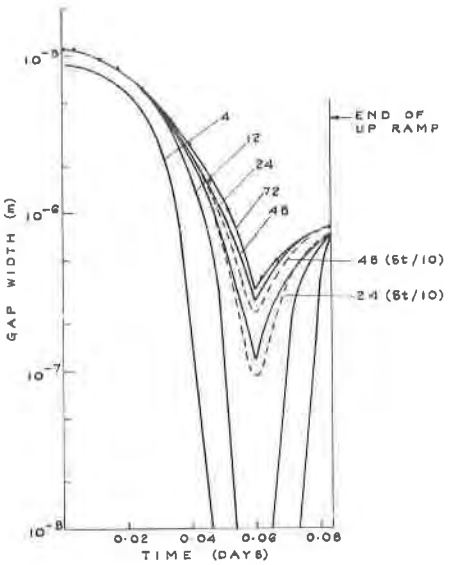


Figure 9 Gap width on the up ramp for various radial mesh sizes. Dotted curves use 1000 time steps on the up ramp.

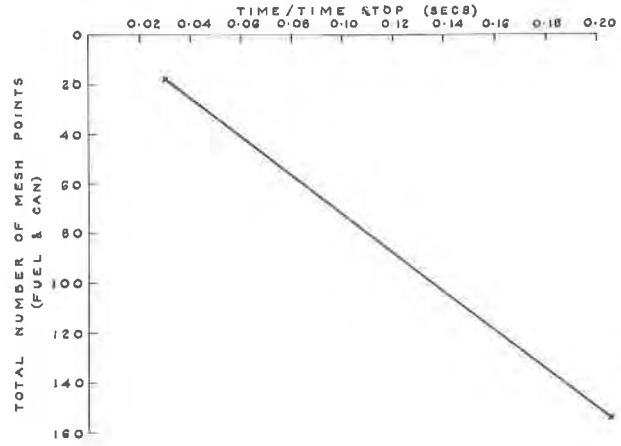


Figure 10 Computing time/time step as a function of the number of mesh points on an IBM 370/165 machine.