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THEORETICAL FUEL ELEMENT MODELLING AT CNEA

by

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ABSTRACT

Computer codes and theoretical developments aiming to model nuclear reactor fuel elements at CNEA are reviewed. The codes PELT, VAINA and BACO for the overall fuel behaviour, as well as the finite element systems ELASTEF, PLASTEF and CTR are described. The influence on the BACO code predictions of including a fuel cracking model is discussed. Also some examples of the calculated fuel cladding contact pressure are shown for different fuel elements. Applications of the finite element systems to calculate the stress concentration at the skids of the Central Nuclear Atucha fuel rods and to predict local thermal effects of PuO_2 particles in a UO_2 fuel are discussed.

RESUMEN

Se presentan los códigos de computación y los desarrollos teóricos conducentes al modelado de combustibles nucleares llevados a cabo en CNEA. Se describen los códigos PELT, VAINA y BACO para el comportamiento global del combustible, y los sistemas de elementos finitos ELASTEF, PLASTEF y CTR. Se advierte la influencia de incluir un modelo de fisuras del combustible sobre las predicciones del código BACO. También se muestran algunos ejemplos de presiones de contacto entre combustible y vaina calculadas para distintos elementos combustibles. Se discuten ampliaciones de los sistemas de elementos finitos para el cálculo de concentración de tensiones en los patines de los elementos combustibles de la Central Nuclear de Atucha y para la predicción de efectos térmicos localizados en las partículas de $Pu O_2$ en un combustible de UO_2.

1. Introduction

In this paper we shall review the fuel element design and performance computer codes developed at CNEA since 1974. By that time, though some experience in fuel modelling codes development existed in Argentina (1), it was evident, taking into account the local needs, that the decision had to be taken of either multiplying the local effort in own development or buying abroad already developed codes. Tough more dangerous, the first decision was taken. This was based not only on economical reasons but, more important, on the understanding that these very complex codes can only be efficiently used by those who have developed them, specially considering the need for the code modifications inherent to new problems. On the other hand it was clear that in order to keep up to international standards.a large collaboration with groups of international reputation in the field was imperative+.

A theoretical group was formed in 1974 within the Gerencia de Desarrollo (Development Area) aiming to cover the previously mentioned needs. Three main lines were established with the purpose of: 1) developing codes for the overall fuel rod behaviour, 2) developing cedes for the description of localized phenomena in the fuel element and 3) to tackle basic underline theoretical studies regarding the materials behaviour under operating conditions. The first and third line are covered at the Gerencia de Desarrollo in Buenos Aires,where the main effort towards fuel element design and fabrication is concentrated, while for the second one the collaboration of a group already established in Bariloche was obtained. This paper will then summarize some of the achievements reached in this period.

2. Computer codes in use

2.1. Overall behaviour codes

Three codes have been developed in order to cover the overall behaviour of the fuel elements:PELT, VAINA, and BACO. The basic philosophy behind the three codes is equivalent, they model respectively the state of stress and strain in a ceramic heat generating cylinder, in a metal cladding and in a fuel rod section.

+ In this sense we would like to thank the collaboration of J. Matthews, H.Elbel, K. Lassmann, R. Bullough and D.H. Locke.

The first two are used as new model testing codes while the third is used as fuel design and performance analysis code.

The assumptions of axial plane strain and axial symetry allow to reduce the three dimensional stress-strain problem to a modified one dimensional one. At present the following contributions to the state of stress and strain are considered at the codes: elastic distortion, thermal expansion, plastic deformation, creep, gas and solid products swelling, thermal and radiation induced redensification and axial and radial cracking. The materials behaviour allows to neglect the plastic deformation of the ceramic fuel and the swelling, cracking and redensification of the zircalloy cladding, which is used in the argentine present and planned power heavy water reactors. The mechanical description is coupled with a thermal self consistent calculation and a fuel gas release model. (2).

The mathematical description of the mechanical behaviour (3) is based on the assumption that the time variation of the strain in a principal direction (r, θ or z), for a finite but small time interval, can be expressed as a linear superposition of the individual strain variations owed to the previous mentioned mechanisms under a common stress and environment conditions. Each of these strains can be written as an explicit function of the stresses at a given point. The mechanical state is described by those equations for the main strains plus the equilibrium and compatibility relations subject to the appropiate boundary conditions. In order to solve the numerical problem the axial section under study is divided into circular rings and a finite difference scheme is applied. A central difference method is adopted, this should result in a relatively stable system of equations to be solved and it showed, when applied to the thermoelastic problem, better convergence than the forward difference scheme which is used in other codes (4). The non linear system of equations for the stresses in a time interval is linearized through a Taylor series expansion. Whenever the tangential or axial stress at a given ring in the fuel exceeds a on predicting the behaviour of a fuel rod. This example will show the importance of the crack induced distortion on the other physical parameters predicted by the code and it will at the same time give an idea of the codes output and versatility.

The code BACO was run for a section of a CNA (Central Nuclear Atucha) anatural uranium fuel rod, assuming that it generates a constant linear power of 480 w/cm during 100 days and that this power has been reached in half a day of linear increase. The fuel is assumed to be cracked at rings where a tangential or axial main stress of 150 MPa has been reached. The calculated central fuel temperature is 2090ºC at the end of the power ramp and 1960º C at the end of the cycle. The tangential stress, calculated along the pellet radius, is plotted in Fig. 1 at different times of the power cycle +. When a tangential or axial crack is open the corresponding main stress at the ring is assumed to be constant and equal to minus the gas pressure in the rod. It can be seen in Fig. 1 that during the power rise the thermal fuel expansion creates a large tensile stress that is relaxed by tangential and axial cracks opening at the outer rings. The largest tensile main stress is then concentrated at the outermost uncracked ring - see t=0.25 d, Fig.1. When constant power is reached and the point to which the crack has penetrated has significant creep, the stress at the pellet becomes compressive and the crack begins to close. The closing down rate as well as the stress in the innermost rings show a large increment when fuel-cladding contact is reached; in this application the contact has ocurred at 5.6 days. In the curves plotted in Fig. 1 for 5.6 and 100 days of power it can be seen that the large amount of creep in the central region determines an almost hydrostatic state of stress.

In Fig. 2 we compare the tangential stress at the end of the power ramp in the previously described case with an equivalent run but where the pellet was not allowed to crack. We see that the cracking has relaxed the stresses by 3 orders of magnitude. Tough

+It is worthy to remember that the Atucha fuel is a solid cylindrical pellet.

predefined fracture stress it is assumed that the ring is "cracked" in that direction. This implies that instead of solving the system of equations for the corresponding unknown main stress at the ring; this stress is considered as a known boundary condition and the system must be solved assuming an unknown crack strain η in that direction. This strain is considered to be made up of a uniform distribution of infinitesimal cracks, which summed over a path give a finite value for η . If during the time integration η happens to become negative, the crack is assumed to be closed or healed, depending on the temperature at that ring.

The previously described system of linear equations for a given time increment can be solved for the main stresses by direct matrix inversion. A very efficient and fast numerical subroutine developed at Harwell (5) for inverting sparse matrices is used.

The finite difference method was chosen for the above described codes because of the following advantages compared to analytical solutions: i) the possibility of a simple treatment of cracks; ii) the possibility of including the variation of material properties with temperature even if they are non linear; iii) to be able to formulate the time dependence of the problem with explicit components and iv) the possibility of extending the calculation to include the interaction between fuel and cladding using the same numerical scheme.

One of the advantages of these codes is to have chosen the main stresses at each ring as the mathematical system unknowns. This allows to solve the fuel-cladding contact without the need of cumbersome iterative procedures or ansatz for the contact pressure. When the contact is attained the boundary condition of radial stress on fuel and cladding becomes an unknown. This stress, i.e.minus the contact pressure, should satisfy, while the contact is mantained, the equality between radial displacements at the internal cladding and external fuel radii. The corresponding equation for this equality is then explicity added to the system. If at any point in the time integration the contact pressure becomes negative, contact is assumed to be broken.

2.2. Localized phenomena codes

2.2. a) The ELASTEF System of codes for thermoelastic problems.

The purpose of this system of codes (6), named ELASTEF, is to solve elastic and thermoelastic two-dimensional (plane stress or strain and axisymmetric stress) and non homogeneous problems of arbitrary geometric shape, using the finite element method. Isolated points and/or portions of the boundary may be subject to conditions of a wide nature:

a) Concentrated forces and/or distributed loads;
b) Imposed displacements;
c) Elastic boundary reactions; and
d) Combinations of the three previous boundary conditions.

Together with those boundary conditions and a certain previously obtained spatial distribution of temperatures, the computer programs calculate the displacements of the elastic system with respect to the coordinates. By using such displacements, strains, stresses and equivalent (von Mises) stresses are obtained at every point of the material under study..

These programs employ triangular finite elements of uniform thickness for the cases of plane symmetry, and annular elements of triangular section for the axisymmetric ones. Within each element, linear interpolation functions are used. Each of them characterized by constant values of the Young Modulus, Poisson ratio and temperature,

2.2. b) The PLASTEF codes for thermoelastoplastic problems.

These are general code which simulate the thermoelastoplastic behaviour of materials using the finite element method (7). They can be used for technological parts of arbitrary shape, where the plane stress and strain, or axisymmetric stress can be solved for given histories of loads and temperature, and for any strain-hardening law. Spontaneous unloadings at any point of the material are automatically taken into consideration.

The programs are based on the incremental initial-stress method. For each increment of loads and temperature, a thermoelastic problem is solved with fictitious initial stresses and the results, which have been obtained from the equilibrium conditions are stored.

The problem is then solved by means of an iterative algorithm modifying the initial stresses, until the laws of plasticity are fulfilled within an acceptable error bound, the iteration process is then interrupted. The Levy-Prandtl-Reuss criterium of plasticity has been adopted.

For each increment of load, the corresponding thermal strains are calculated with the temperature distribution obtained from the auxiliary code CUARM (8), and the thermoelastic incremental problem is solved with some of the routines of the ELASTEF System.

The program presently uses linear triangular elements, It has a total high speed memory requirement of about 100 Kbytes, and it also needs auxiliary storage disks. This capacity permits triangular nets of about 300 elements and 200 nodes.

2.2. c) The CTR code for difussion problem.

This code (9) calculates a numerical solution of the transient quasi-harmonic equation in two independent space variables (plane and axial symmetry) in domains of arbitrary shape, for the initial value problem with non homogeneous Dirichlet and Neumann boundary conditions.

The procedure is mathematically framed within the Galerkin-Faedo method. The physical space is discretized with linear triangular elements and the time variable by finite differences, using a Crank-Nicolson scheme.

The capacity of the program, for a total high memory requirements of 100 Kbytes, allows for a mesh of about 1100 elements and 800 nodes.

3. Examples of code applications

3.1. Influence of a cracking model on predicting the fuel performance.

The amount of information produced by the codes used to predict the overall fuel behaviour is so enormous that it is difficult to choose a representative example. We shall discuss in this section the influence of allowing for a model of fuel cracking the creep has already relaxed the stress at the innermost rings in the uncracked pellet the allowance for cracking largely relaxes those stresses in that uncracked region. Also the radial expansion of the pellet is larger by 11% if cracking is allowed; this difference implies in turn that the central temperature of the fuel is 84º C smaller (2092ºC against 2176ºC) at this point. As the uncracked fuel is hotter it emits more gases and the calculated gas pressure during the pewer cycle is then much larger in this case than in the case where the pellet is allowed to crack.

We wish to finish this example by emphasizing that the crack structure is strongly correlated with the stress-strain state of the material. This means that the results of the application where cracking is not permitted, may not be extrapolated to give the behaviour of the cracked material. For example in that application at the end of the power ramp the cracking tension of 150 MPa is reached at a radius of 0.82 r_{ext} - Fig.2 - while the tip of the crack is located at the radius R= 0.48 r_{ext} in the application where cracking is allowed for.

3.2. Contact pressure.

In this example we wish to show different applications of the unidimensional codes where fuel-cladding contact is reached under quite different conditions. One is an application to a prototype 4% enriched fuel with a very small (0.005 cm) fuel-cladding gap, where the fuel-cladding contacts is reached during the power ramp - constant power is assumed to be reached in 0.5 days. The second is the application to the CNA fuel element previously discussed. Here the contact is reached after 5.6 days of constant power. The evolution of the contact pressure is shown in Figures 3a) and 3b) for either application. We see that in the first case, where plastic deformation of the cladding is reached during the ramp, when constant power is attained a large relaxation of the contact pressure arises. This value of the pressure shows afterwards a very smooth increase during the irradiation. When the contact is established at constant power - Fig. 3b) - the contact pressure reaches very soon an equilibrium value which then also evolves very smoothly with irradiation. However in this case no initial maximum in the pressure occurs.

3.3. Thermoelastic analysis of the Atucha fuel cladding in the skids region.

A two dimensional thermoelastic analysis has been made for an axial section of the CNA fuel cladding which contains the skids welded to the rod (10). Whenever the gap between the skids and the fuel rod separator's support is closed, this support reacts elastically to the radial cladding expansion. For different rods of the fuel element, the internal pressure which allows the stress at the cladding to overcome the zircalloy yield stress is calculated as a function of the initial cladding-support gap. A fuel cladding of the real dimensions as well as a reduced wall thickness one have been considered. The external pressure is taken as a calculation parameter while the temperature spatial distribution has been calculated by solving the heat conduction equation along the fuel element for a given power level.

The calculations are performed with two computer codes based on the finite element method: the NOLICUARM (8), which solves the non linear heat conduction equation and the ELASTEF 3 - which belongs to the ELASTEF System - for obtaining the thermoelastic stresses.

Level curves for the equivalent (von Misses) stress in the sector of the cladding are shown in figure 4. In this example internal and external pressure over the cladding is included while the skids are assumed to be in contact with the separator support.

3.4. Evaluation of the local effects produced by particles of PuO_2 in UO_2 fuel rods.

One of the projects of the Gerencia de Desarrollo in CNEA is to study the behaviour and performance of natural UO_2 fuel elements enriched with plutonium. Within this fuel element, the plutonium should form PuO_2 solid solution inside the UO_2 pellets,in a wide range of concentrations. However if the solutions are obtained by mechanical mixing of the oxides., PuO_2 islands are formed in the UO_2 matrix. These islands may be the source of several problems in the fuel behaviour, perhaps the most important is the overheating of the matrix in the particles neighbourhood.

A detailed study of the thermal effects produced by PuO_2 particles in the UO_2 matrix is important for the specification of their permissible size. A portion of the fuel rod with PuO_2 particles in several places inside it was studied. The spatial distribution of temperature and heat flux was calculated for a certain power level of the reactor as a function of the particles size (11). The stationary non linear equation of heat conduction with temperature dependent conductivities - has been solved by means of the finite element AXICUARM code (8). The influence of different size PuO_2 islands on the temperature for a fuel element similar to the CNA fuel but Pu enriched is shown in figures 5 and 6.

4. Theoretical underline work.

In order to support and improve the mathematical description of the fuel behaviour under irradiation it is necessary to understand the material problems of their components. Only this understanding can provide some confidence in the extrapolated behaviour necessarily far from the laboratory conditions. The work in this area aims, for the time being, to the understanding of the zircalloy cladding properties under irradiation, with special emphasis on the influence of the material anisotropy on the mechanical behaviour under irradiation. In this context theories of irradiation growth (12) and creep (13,14) are being developed as well as more basic work on simulation of intrinsic defects configuration (15). The radiation growth theory (12) allows for example to correlate measured growth with microestructural parameters (like loops and network dislocation density) and the irradiation flux and dose for a cold worked zirconium alloy cladding or structural core component.

5. Conclusions.

The computer codes and some theoretical developments tackled at CNEA in order to model and improve the understanding of the nuclear fuel performance under irradiation have been reviewed. The computer codes are used at present for providing a theoretical back up to the operating decisions related to the fuel element at the CNA (Central Nuclear Atucha) and for relating fuel irradiation experiments with laboratory predictions. Also Argentina will construct in the near future the fuel elements for the CNA and the CANDU type CNE (Central Nuclear Embalse) heavy water thermal reactors. It is imperative therefore to adquire a deep understanding, both theoretical and experimental, of the fuel elements and materials behaviour under irradiation. This understanding will in turn provide a fuel design capability.

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FIGURE CAPTIONS

Figure 1 ; Tangential stress as a function of the fuel radius for a CNA fuel at different times of a power cycle.

Figure 2 : Tangential stress at the end of the power ramp for a CNA fuel. The full curve corresponds to the fuel that was allowed to crack, while in the dotted line the cracking was not allowed.

Figure 3a: Contact pressure for a prototype 4% enriched fuel as a function of the irradiation time.

Figure 3b: Contact pressure calculation for a CNA fuel.

Figure 4 : Level curves of the equivalent (von Mises) elastic stress in a sector of the Atucha fuel rod cladding. External and internal pressure, spatial temperature distribution, and reaction of the separator's support are included in the calculation.

Figure 5 : Radial temperature distribution in a UO_2 fuel rod with a PuO_2 particle on its axis. The particle diameters are taken as parameter.

Figure 6 : Radial temperature distribution in a UO_2 fuel rod with a PuO_2 particle near the cladding . The particle diameters and positions are indicated for each case.

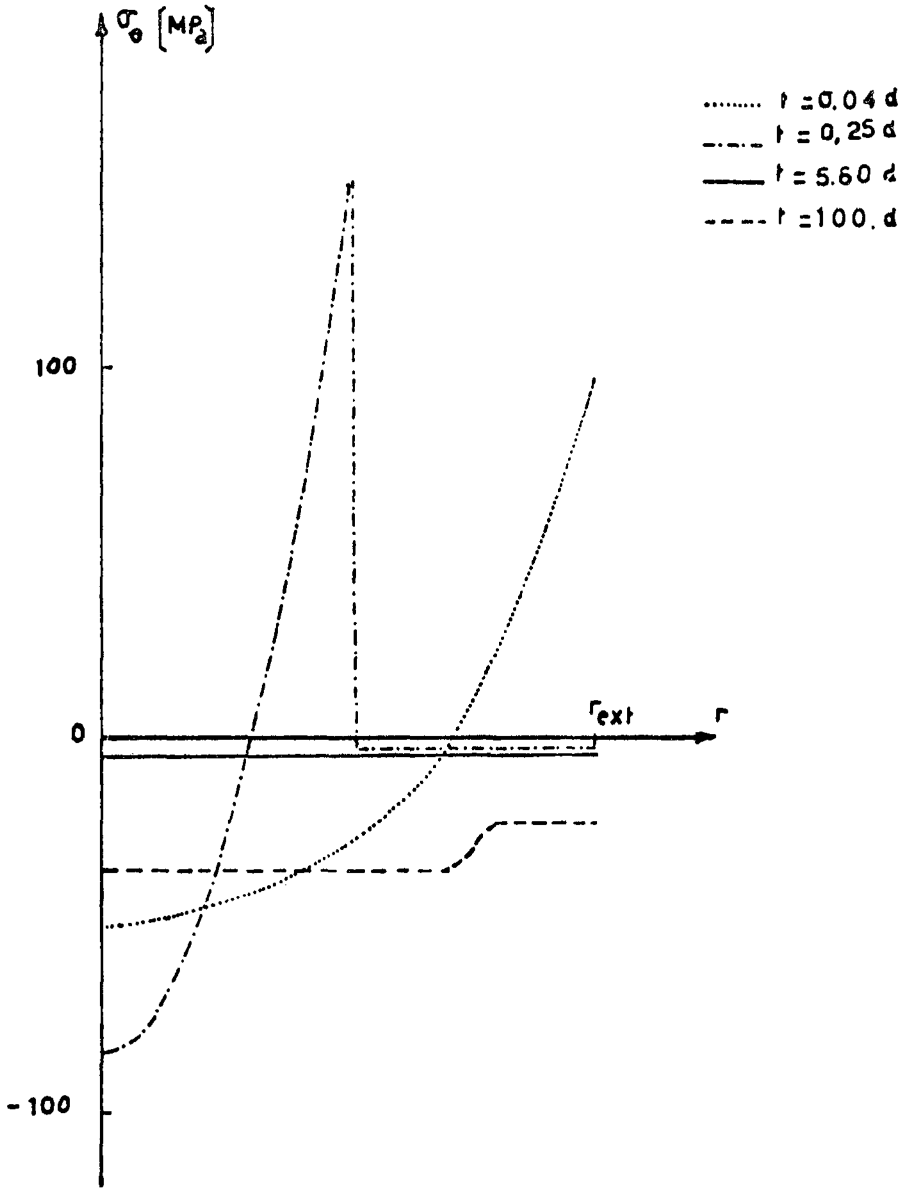

FIGURE 1

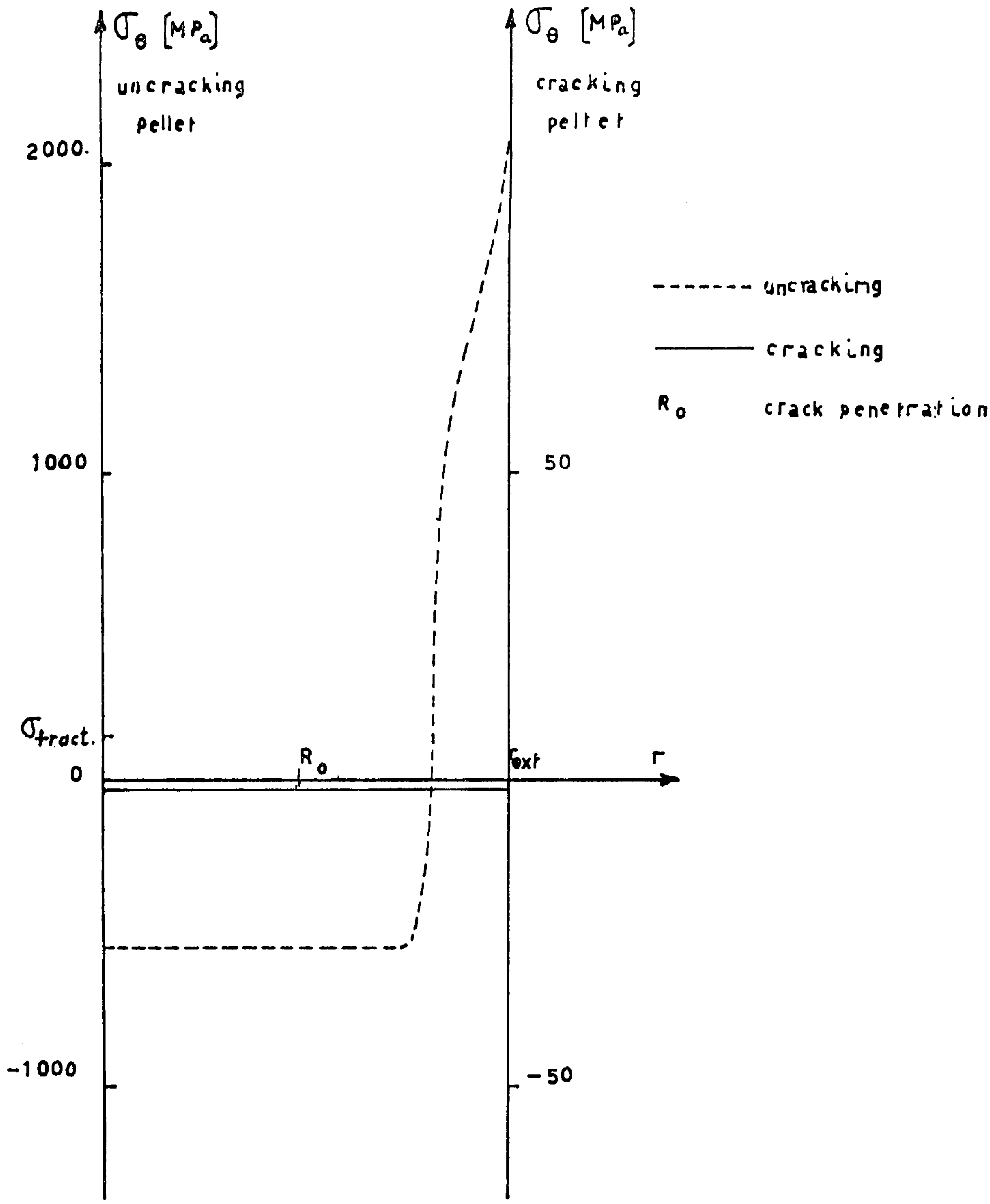
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FIGURE 2

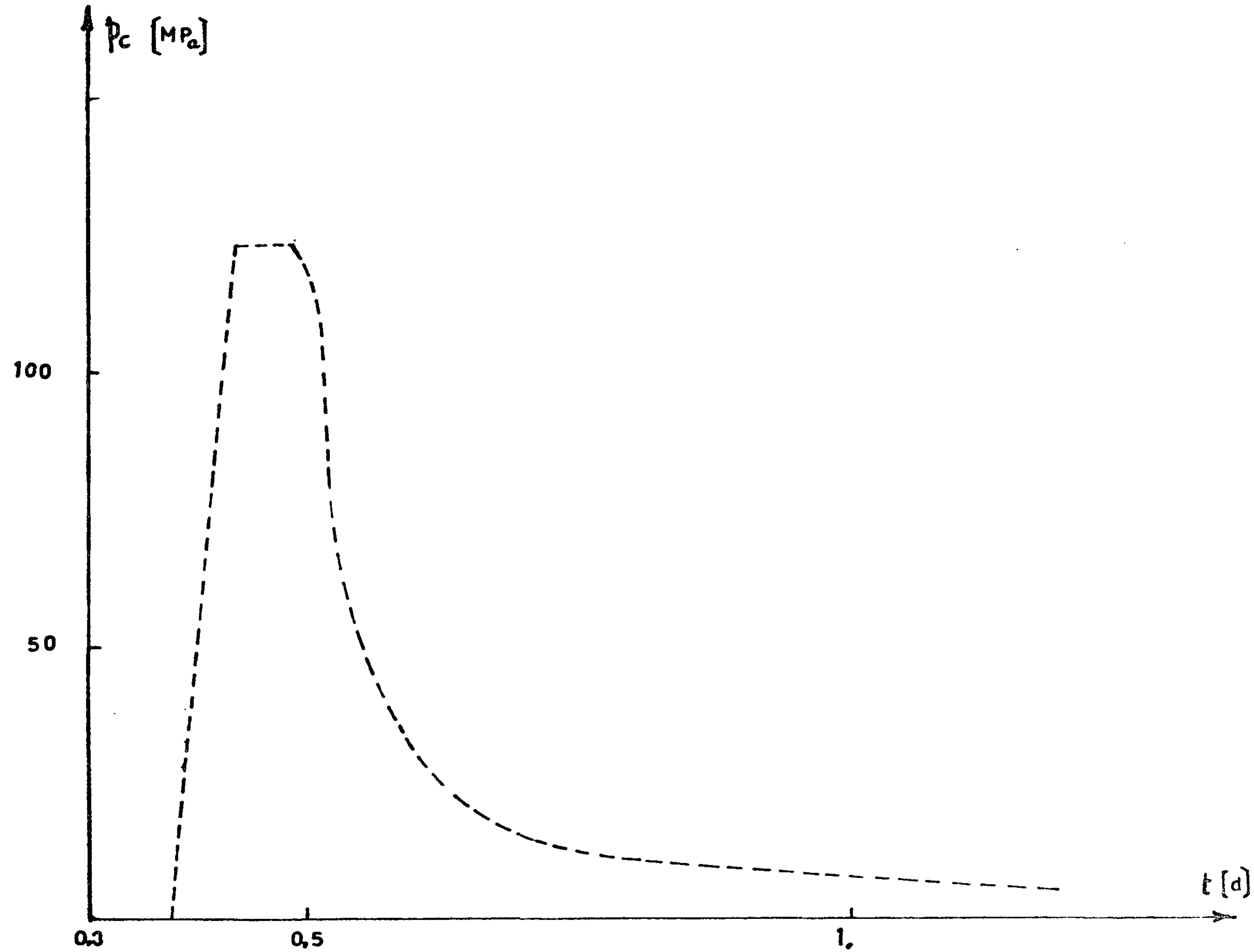

FIGURE 3 a)

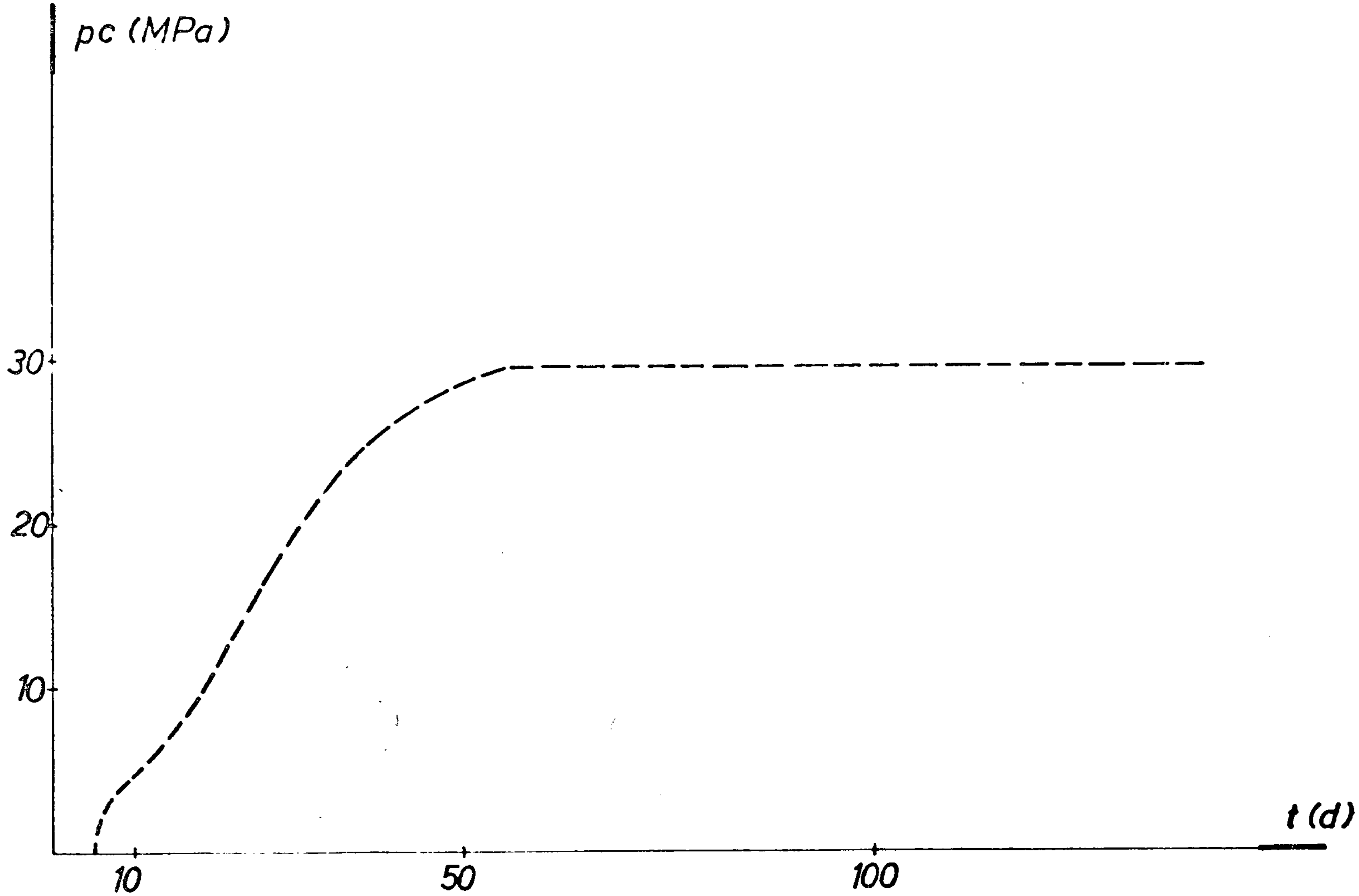

FIGURE 3 b)

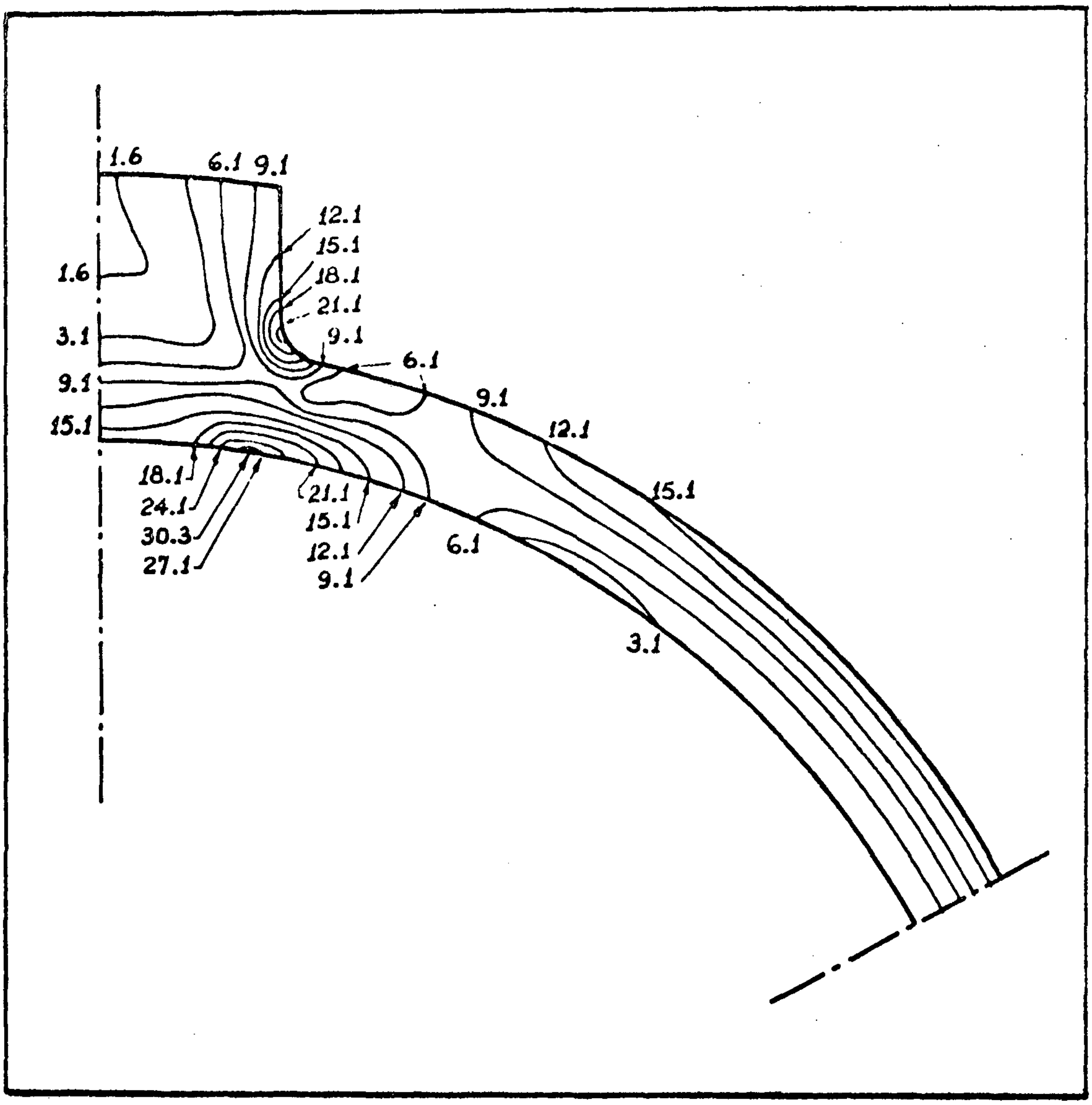
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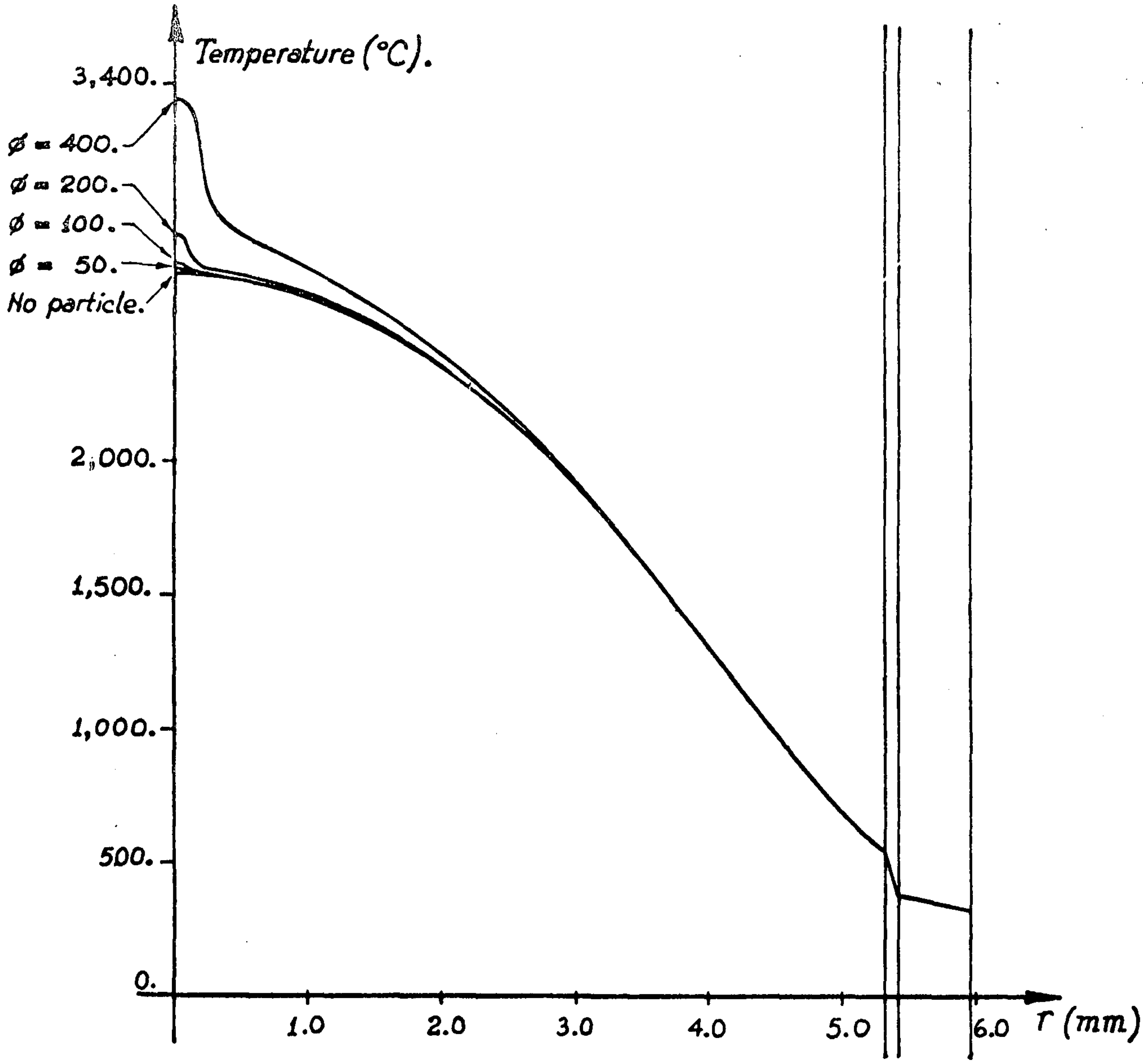
FIGURE 4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ø = 200.
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No particle.
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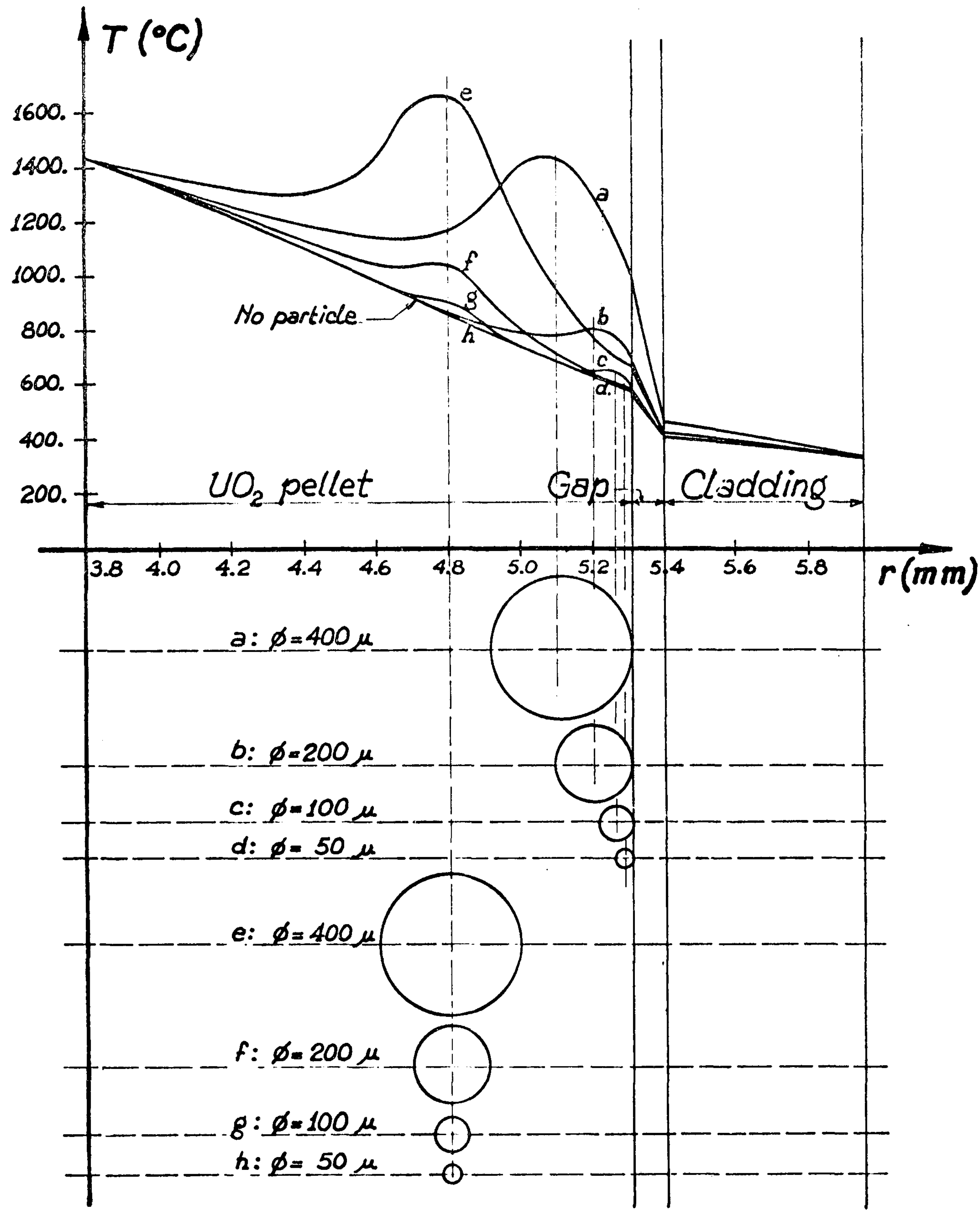
6.0
r (mm)

FIGURE 5


T (°C)
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Gap
Cladding
3.8
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4.4
4.6
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5.0
5.2
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5.6
5.8
r (mm)
a: ϕ=400 μ
b: ϕ=200 μ
c: ϕ=100 μ
d: ϕ= 50 μ
e: ϕ=400 μ
f: ϕ=200 μ
g: ϕ=100 μ
h: ϕ= 50 μ

FIGURE 6