Specialists' meting on transient two-phase flow.
Toronto, Ontario, Canada, 3-4 August 1976

CEA-CONF--3831

FR7800145

DEVELOPMENT OF NUMERICAL METHODS FOR THERMOHYDRAULIC PROBLEMS IN REACTOR SAFETY

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ABSTRACT

Numerical methods are being developed for the LOCA calculation ; the first part is devoted to the BERTHA model and the associated characteristic treatment for the first seconds of the blowdown, the second part presents the problems encountered for accounting for velocity difference between phases. The FLIRA treatment of the reflooding is presented in the last part : this treatment allows the calculation of tne quenching front velocity.

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DEVELOPMENT OF NUMERICAL METHODS FOR THERMOHYDRAULIC PROBLEMS IN REACTOR SAFETY

Introduction

At present time, numerical methods are developed for the resolution of the thermodynamics problems appearing during the loss of coolant accident for pressurized water reactors.

The first part of this report is devoted to the beginning of the blowdown, when the non equilibrium of the temperature of the two phases is the most important phenomenon : this phase is treated by a five-equation model.

The treatment of the velocity difference between the phases is the subject of the second part of this work: various methods are presented and compared.

The last part is devoted to the reflooding : a special model has been developed for the thermohydraulics treatment and the speed of the quenching front is determined by a detailed heat conduction calculation.

Blowdown Calculation

Blowdown is a highly irreversible phenomenon: thus the double phase mixture is out of equilibrium, the liquid temperature may be far from the saturation temperature and a delay may appear before vaporisation.

The standard homogeneous model without slip is used to describe unidimensional flow and two equations are added :

- the first describes the liquid phase thermal non-equilibrium
- the second one simulates the delay of the vapor phase growth (the vapor is at saturation temperature).

Thermohydraulic equations

The three balance equations are used :

$$\frac{D\rho}{Dt} + \rho \frac{\partial u}{\partial z} = - \frac{\rho u}{A} \frac{dA}{dz} \qquad (1)$$

$$\rho \frac{Du}{Dt} + \frac{\partial p}{\partial z} = - \frac{f\rho\, u|u|}{2\, Dh} - \rho g \cos\theta \qquad (2)$$

$$\frac{DH}{Dt} - \frac{1}{\rho} \frac{Dp}{Dt} = Q \qquad (3)$$

Where

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u \frac{\partial}{\partial z}$$

The fourth equation is to account for the liquid non-equilibrium, it states that :

$$\frac{Dh_\ell}{Dt} - \frac{1}{\rho_\ell} \frac{Dp}{Dt} = Q_\ell + \phi\, S_{\ell v}\ (z,\ t) \qquad (4)$$

Where Q_ℓ is the part of the thermal flux Q directly transmitted to the liquid, Φ is the thermal flux exchanged between the liquid and vapor

phases and $S_\ell v\ (z,t)$ is the specific exchange surface.

The vaporisation delay is treated by the fifth equation :

$$\omega \frac{D\Phi}{Dt} + \Phi = h\ (T_{sat} - T_\ell) \tag{5}$$

$$h_v = h_{v_{Sat}}(p) \tag{6}$$

ω is considered as a relaxation parameter to be correlated by experimental results and h is the usual exchange coefficient.

This model had been previouly used in [1].

This quasi linear partial differential system of equations is hyperbolic : it may be written under the symbolic form :

$$A \frac{\partial \vec{Y}}{\partial t} + B \frac{\partial \vec{Y}}{\partial z} = \vec{F}$$

The $\vec{Y}$ vector describes the flow state, it has five components : u, p, h_ℓ, X, Φ ; it can be shown that the equation :

$$\det\ (B - \lambda A) = 0$$

has always three solutions : $\lambda = u$ which is threefold degenerate and $\lambda = u \pm c$, where c is given by :

$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_{adia,\ S_\ell,\ h_{Sat}}$$

c is the propagation velocity of a small perturbation ("sound velocity") ; the derivative being computed without heat exchange ($\delta Q = 0$), with constant liquid entropy and the enthalpy being equal to $h_{Sat}(p)$.

The detailed expression giving c is rather intricate and the computed values are slightly lower than those obtained with the frozen model.

Numerical resolution

The system being hyperbolic, the method of characteristic has been chosen for the numerical resolution : this method provides accurate results for fast pressure transients.

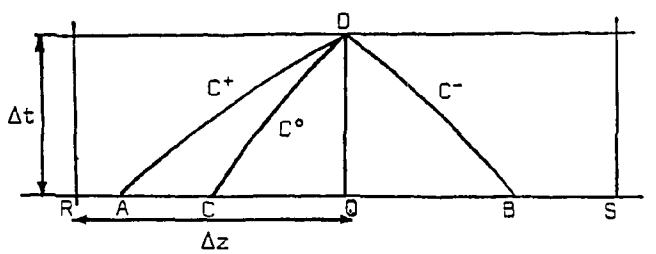
By projection over the characteristic directions $u \pm c$, the Eqs 1 and 2 give :

$$\rho \frac{D^{\pm}u}{Dt} \pm \frac{1}{c}\frac{D^{\pm}p}{Dt} = \mp \frac{\rho u c}{A}\frac{dA}{dz} - \frac{f\rho u|u|}{2D_h} - g\cos\theta$$

$$\pm Q c \rho^2 \frac{(\rho_v - \rho_\ell)}{\rho_v \rho_\ell (h_\ell - h_v)} \mp c(Q_\ell + \varphi S_{\ell v}) \frac{(1-X)\rho^2}{\rho_\ell}\left(\frac{1}{\rho}\left(\frac{\partial \rho_\ell}{\partial h_\ell}\right)_p + \frac{\rho_v - \rho_\ell}{\rho_\ell (h_\ell - h_v)}\right) \qquad (7)$$

The $\frac{D^{\pm}}{Dt}$ symbol denotes derivatives along characteristics $u \pm c$.

A mesh grid is chosen in the (z, t) plane ; the solution at point P is determined by the knowledge of the function on the strip RS



These functions are known as initial conditions or from the calculation at the previous time step.

Eqs (3) - (7) form a differential system which is discretized ; the time step is chosen to verify the condition

$$\Delta t < \frac{\Delta z}{(c + |u_{max}|)}$$

By this condition, the resolution is explicit and stable.

The speed of the calculation and the accuracy of the results depend on the choices of some options :

- Approximation of the characteristics curves : an exponential representation of these curves is used to improve the accuracy.

- Function values at the points A, C, B : X, h_ℓ, Φ are linearly interpolated between R and Q (resp. Q and S).
For p and u , Eqs 1 and 2 are numerically integrated on RA or BS.

- Choice of the values of functions needed for the calculation of the matrix elements

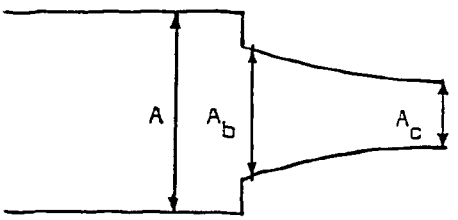
Some of the functions used are fastly varying, i.e. Φ which depends on $T_{Sat}(p)$: in this case a first order representation is used.

$$T_{Sat}^{P} = T_{Sat}^{A} + (P_p - P_A)\left(\frac{d\,T_{sat}}{dp}\right)$$

- Beginning of boiling

In the plane (z, t), the limit of boiling is a singular line for the functions which vary very rapidly in the neighborhood : a special treatment is used for the characteristic curve to limit the unaccuracy.

- Treatment of the breach



A contracted section is determined by the correlation :

$$\frac{A_c}{A_b} = 0.63 + 0.37 \left(\frac{A_c}{A}\right)^3$$

For the treatment of the breach, a sudden variation of the section from A to Ac is supposed and steady state conservation laws are use for flow, rate, impulsion and total energy.

Organisation of the code :

The modular code IALEMOS is being developed based on this model, for the calculation of the blowdown of a PWR : the total system can be described by its elements which are treated by the method presented here.

An example of the results obtained is presented on Fig. 1 : experimental and numerical results are compared for the blowdown of the CANON experiment [1].

Treatment of non equal phase velocities

For two-phase flow at lower pressures, the liquid and vapor will travel at different velocities. To account for this, the three conservation equations can be written for a two-phase mixture having liquid velocity u_ℓ and vapor velocity u_v [2]. This means an extra variable (for example, the relative velocity $u_r = u_v - u_\ell$) which requires a new relation to determine it.

The velocity difference may be given by a correlation, for instance the void fraction, as a certain approximate function of flow variables X, P and G . This implies a relation between u_v and u_ℓ. Correlations proposed from data for steady-state flow are sometimes introduced into the transient two-phase conservation equations (e.g. [3]).

It is well known that these equations, particularly at low pressures and high mass flow rates, may not have all three characteristic velocities real [4-6] . With complex characteristics, numerical solution by the method of characteristics is of course impossible.

We have found that the appearance of complex characteristics is not due to the velocity difference itself, but rather to its rate of variation with the flow variables, as implied by the derivatives of the correlation. Note that to calculate the characteristic velocities, the conservation equations must be expanded in the dependent variables chosen (for instance X, P, G), and this will involve taking derivatives of the correlation. Since the correlation function itself is empirical and not often precise, this is somewhat disquieting. In fact, we have found that derivatives of the correlation strongly influence the characteristic velocities calculated.

Since characteristics have physical interpretations (signal propagation, choked flow), and since the derivatives of a correlation are far from being grounded in physical reasoning, one may ask whether these derivatives could not better be determined by separate physical arguments. As an experiment, we tried imposing $du_r = 0$; that is, we assume small changes in the flow variables for which u_r does not change. This hypothesis is for local, instantaneous changes only. Numerically, we found that expanding differential terms using $du_r = 0$ leads to three real characteristics for all flow conditions of interest, both for water and sodium.

Unfortunately, this fact is difficult to incorporate in an overall consistent flow model. Mathematically, posing $du_r = 0$ in the expansion of differentiated terms is the same as adding u_r as a new flow variable. Then to be fully consistent we must expand each conservation equation to include terms in $\partial u_r/\partial t$ and $\partial u_r/\partial z$ as well as the derivatives of X, P, G. Numerically we found that these extra terms can be non-negligible. Thus to

complete the problem (without using derivatives of a correlation) we can : (1) Introduce a relaxation equation for u_r , for example

$$Du_r/Dt = (u_r^{*} - r_u)/\tau ,$$

where u_r^{*} is the correlation value. This type of equation has the advantage of giving the same three real characteristic velocities obtained from the three conservation equations plus $du_r = 0$. However, physical justification may be lacking , furthermore, this equation plus the three conservation equations may have a multiple characteristic with an insufficient number of projection eigenvectors, another obstacle to numerical MOC solution. (2) Alternatively, pose some other differential equation for u_r. In general this will lead to a fourth degree equation for four characteristic velocities, whose numerical solution becomes too time-consuming.

Thus the method of characteristics seems ill-suited for numerical two-phase flow calculations with unequal phase velocities. The imolications for the two-phase flow models themselves should also be examined.

It has been suggested that the appearance of complex characteristics need not be regarded as unphysical. We disagree, for several reasons. First, the change from all real to some complex characteristics changes the nature of the problem. Signal propagation is partly lost ; in passing to a state where characteristics are complex, two of the originally real characteristics (the middle and either the forward or backward characteristic) must approach and coincide, which means suppressing wave propagation at finite speeds either upstream or downstream. All this might be acceptable if not for the observation that these changes depend on highly arbitrary circumstances. Roughly similar correlations may display complex characteristics in widely different conditions. Furthermore, even if characteristics stay real, their sensitive dependence on derivatives of the correlation makes the results seem arbitrary.

In conclusion we feel that a two-phase flow model based on three conservation equations plus an empirical steady-state correlation for velocity

differences between the phases is not only unsuitable for MOC methods but fundamentally suspect for rapid transients. (Of course, it should be acceptable for slower transients insofar as it works for the steady state). We think it will be necessary to add a vapor phase momentum equation to determine the velocity difference, and are developing an implicit finite difference solution method for such a model.

Reflooding calculations

Thermohydraulical Equations

Fuel rewetting calculations with the code FLIRA II are based on a detailed physical description with different thermohydraulic flow models in the wetted and unwetted portions, taking into account radiation heat transfer and 2D heat conduction calculation in the vicinity of the wetting front.

In the wetted region it is assumed that :

- the wall is in contact with the liquid phase ;
- boiling occurs before the liquid reaches saturation temperature (non-equilibrium state) ;
- boiling is nucleate or undispersed or annular flow ;
- heat transfer by radiation is negligible ;
- the energy exchange between the two phases is proportional to their temperature and to the quality X which, for low values, may be assumed proportional to the inter-phase contact surface area.

The main unknowns used are :

- pressure p(z,t)
- mass flow-rate : G(z,t)
- mean enthalpy of the fluid : H(z,t)
- enthalpy of the liquid phase : $h_\ell(z,t)$

The set of equations governing the behaviour of the fluid in the wetted region may be written :

- continuity $\quad \frac{\partial \bar{\rho}}{\partial t} + \frac{\partial G}{\partial z} = 0$

- momentum $$\frac{\partial G}{\partial t} + \frac{\partial\, v'' G^2}{\partial z} + \frac{\partial p}{\partial z} = - \frac{f\, G|G|}{2\bar{\rho}\, Dh} - \bar{\rho} g$$

- energy $$\frac{1}{v''}\frac{\partial H}{\partial t} + W \cdot \frac{\partial p}{\partial t} + C \cdot \frac{\partial h_\ell}{\partial t} + G \frac{\partial H}{\partial z} = \frac{\phi\, \chi}{s}$$

- liquid non-equilibrium

$$\rho_\ell (1-\alpha) \frac{\partial h_\ell}{\partial t} + G(1-X) \frac{\partial h_\ell}{\partial z} = \frac{\phi_\ell\, \chi}{s} + K_1 (H-h_\ell) \frac{(h_{sat}-h_\ell)}{C_p}$$

The unwetted model is based on the following assumptions :

- the steam is against the wall and receives energy from it by conduction ; it is therefore superheated ;
- the liquid receives energy from the wall by radiation transfer and from the steam by convection ;
- the hypotheses governing the interface energy exchange are the same ; however the term proportional to the exchange surface must be corrected for high X values ;
- radiation transfer between the wall and the water and steam is calculated by a two flux method. For this calculation we assume that the steam is gray and the wall is also gray and diffuse. Water droplets are an absorbing and diffusive medium for radiation ;
- the energy received by the liquid phase is divided into two fractions ; the first one, proportional to the difference between the liquid enthalpy and the saturation enthalpy, heats the liquid ; the other vaporizes it ; to the four (upsteam) unknowns, we add the steam enthalpy h_v and the steam flux ϕ_v.

The continuity and momentum equations are the same as upstream.

The four other equations are :

Energy :

$$\frac{1}{v''}\frac{\partial H}{\partial t} + w \frac{\partial p}{\partial t} + C \frac{\partial h_\ell}{\partial t} + E \frac{\partial h_v}{\partial t} + G \frac{\partial H}{\partial z} = \frac{\phi\, \chi}{s}$$

Liquid non-equilibrium :

$$(1-\alpha)\ \rho_\ell \frac{\partial h_\ell}{\partial t} + G\,(1-X)\,\frac{\partial h_\ell}{\partial z} = \frac{\phi_\ell\, X}{S} + K_2(H-h_\ell)\left(\frac{h_v-h_g}{C_v} + \frac{h_{sat}-h_\ell}{C_p}\right)\left(\frac{h_{sat}-h_\ell}{h_{sat_o}-h_{\ell_o}}\right)$$

Steam non-equilibrium :

$$\rho_v\,\alpha\,\frac{\partial h_v}{\partial t} + G\,X\,\frac{\partial h_v}{\partial z} = \frac{\phi_v\, X}{s} + K_2(H-h)\left(\frac{h_\ell-h_{sat}}{C_p} + \frac{h_g-h_v}{C_v}\right)$$

Radiation heat transfer to the steam :

$$\phi_v = \phi - \phi_{rad.\ell}$$

Motion of the quenching front

The FLIRA II code includes the calculation of the motion of the quenching front and the heat fluxes exchanged between the fuel element and the reflooding fluid. The resolution of the thermohydraulic equations provides the heat flux exchanged between the fluid and the cladding ; a two-dimensional, time dependent, heat conduction calculation defines the temperature of the fuel. An iterative scheme couples the two parts of the calculation to obtain the position of the quenching front ; this front divides the channel into two parts, upstream and downstream, for which the thermohydraulic equation of the FLIRA I model are used. The quenching front is assumed to be the point where the clad temperature is equal to the Leidenfrost temperature or any temperature correlated on local thermohydraulical parameters.

Figure 2 presents the data flow chart of FLIRA II and the iterative scheme used.

The 2D heat conduction calculation is limited to a short strip near the quenching front (about 1 cm) ; in the other part, the computation is limited to an energy balance.

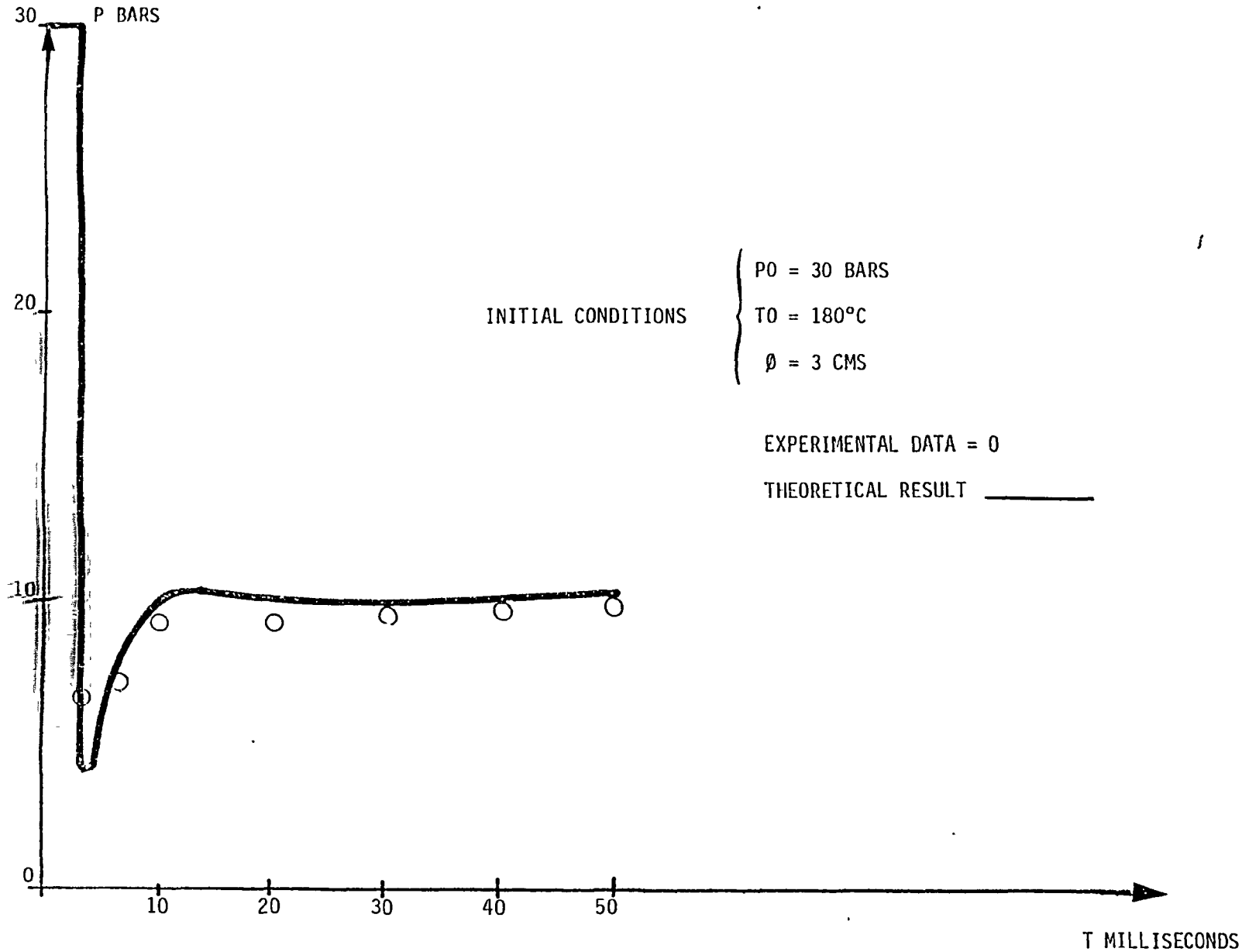


Figure 1 : BLOWDOWN OF THE CANON EXPERIMENT

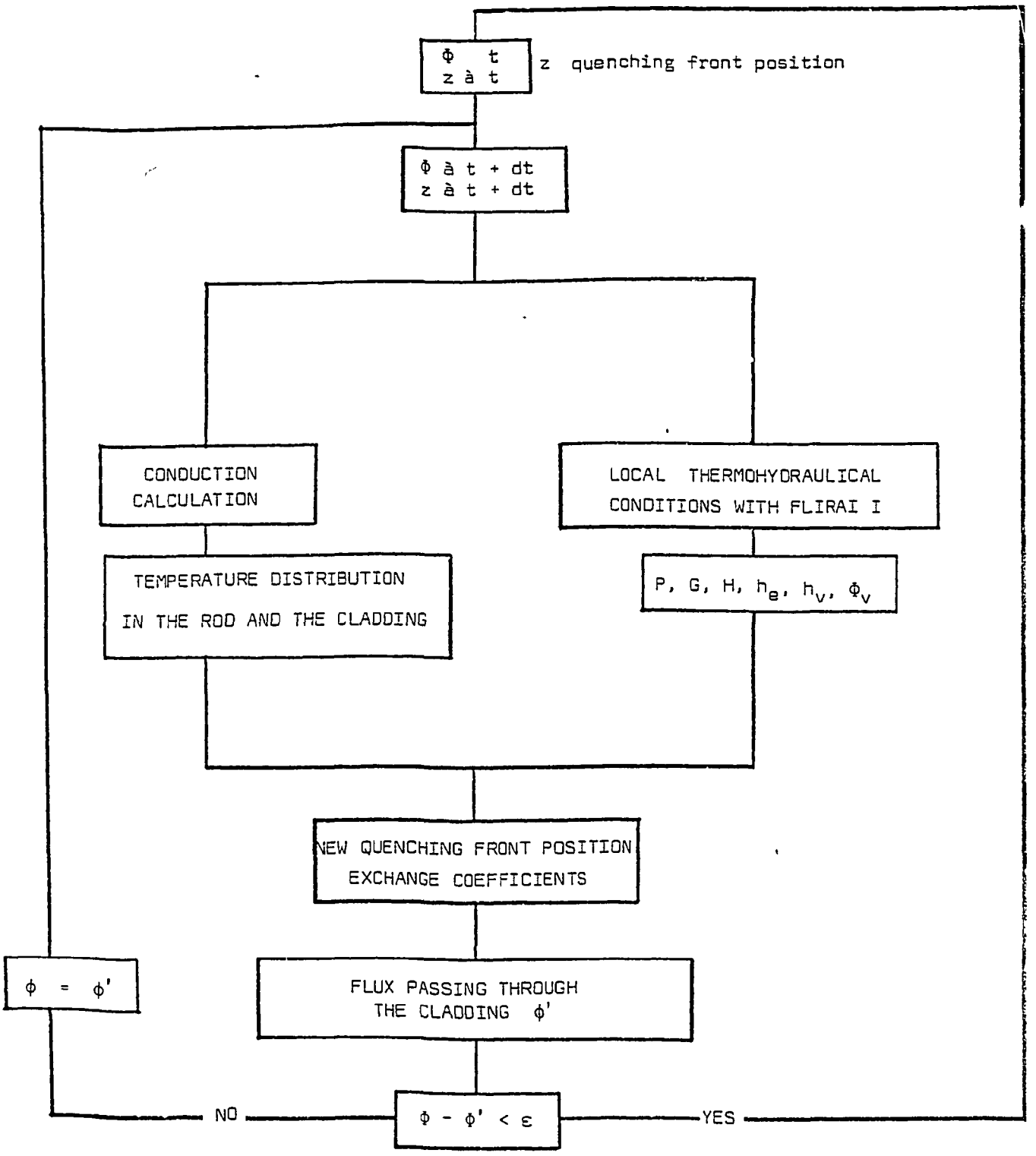

Φ t
z à t
z quenching front position
Φ à t + dt
z à t + dt
CONDUCTION CALCULATION
LOCAL THERMOHYDRAULICAL CONDITIONS WITH FLIRAI I
TEMPERATURE DISTRIBUTION IN THE ROD AND THE CLADDING
P, G, H, h_e, h_v, Φ_v
NEW QUENCHING FRONT POSITION EXCHANGE COEFFICIENTS
$\phi = \phi'$
FLUX PASSING THROUGH THE CLADDING ϕ'
NO
$\Phi - \phi' < \varepsilon$
YES

Figure 2

Numerical calculations

A. Thermohydraulical computation

The quenching front divides the problem into two parts upstream and downstream where the equations to be satisfied are different.

At the quenching front, the thermohydraulical functions are assumed to be continuous but their derivatives are discontinuous.

Formally, the equations may be written as :

$$\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial z} = S(z,t)$$

A (z,t) mesh grid is used, f_i^k represents the value of the function at the abscissa z_i and at time t_k.

The time derivative $\frac{\partial f}{\partial t}$ is represented by :

$$\left[\frac{\partial f}{\partial t}\right]_i^{k+1} \rightarrow \frac{f_i^{k+1} - f_i^k}{\Delta t}$$

Two formulae are used for the space derivative according to the $u \frac{\Delta t}{\Delta z}$ ratio.

a) $\quad o < u \frac{\Delta t}{\Delta z} < 1 \qquad \left[\frac{\partial f}{\partial z}\right]_{i+1}^{k+1} \rightarrow \frac{f_{i+1}^k - f_i^k}{\Delta z}$

b) $\quad 1 < u \frac{\Delta t}{\Delta z} \qquad \left[\frac{\partial f}{\partial z}\right]_{i+1}^{k+1} \rightarrow \frac{f_{i+1}^{k+1} - f_i^{k+1}}{\Delta z}$

At the quenching front a special treatment is used.

The resolution is performed timestep by timestep and point by point in the flow direction. An overall iteration is needed when the output pressure is a limit condition.

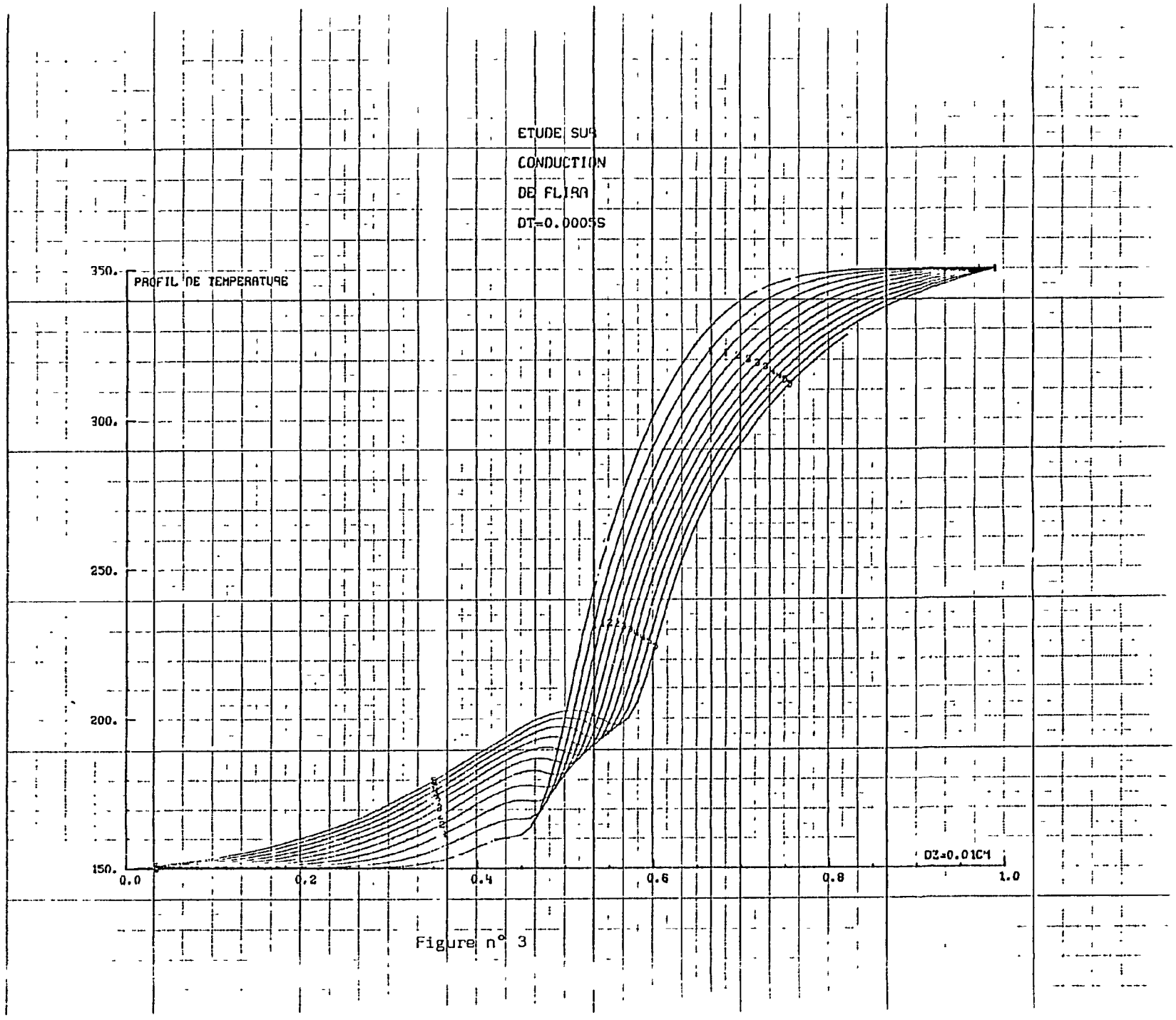

ETUDE SUR
CONDUCTION
DE FLIRR
DT=0.0005S
PROFIL DE TEMPERATURE
350.
300.
250.
200.
150.
0.0
0.2
0.4
0.6
0.8
1.0
DX=0.01CM

Figure n° 3

B. Heat conduction calculation

A standard implicit discretization of the conduction equation is used for the two dimensional, time dependent treatment. The shape of heat flux used as limit condition requires a very refined mesh grid in z (about 0.01 cm) and the corresponding time step is about 0.01 s.

This detailed calculation is to be compared to the mesh grid used for the thermohydraulical calculation where the sace mesh is about 10 cm and time step about 5 s.

C. Numerical results

On Figure 3, are plotted the temperature distribution at some time steps during a refined conduction calculation.

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