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UN NOUVEAU COUPLAGE DE CODE 3D DE THERMOHYDRAULIQUE THYC ET DU CODE DE THERMOMECANIQUE CYRANO3 POUR LES CALCULS DE REP

A NEW COUPLING OF THE 3D THERMAL-HYDRAULIC CODE THYC AND THE THERMO-MECHANICAL CODE CYRANO3 FOR PWR CALCULATIONS

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SYNTHÈSE :

EDF, en sa qualité de compagnie électrique nationale, est responsable de cinquante-quatre REP, ce qui signifie qu'un grand nombre de calculs de comportement neutronique sont nécessaires pour la sécurité en fonctionnement normal et en cas d'incident, ainsi que des calculs prospectifs d'analyse des accidents graves.

Entre tous les paramètres, la température du combustible a une importante influence sur la réactivité du cœur, en raison de l'effet Doppler qui se produit sur les sections.

La plupart des codes neutroniques appliquent une méthode directe pour calculer la température moyenne du combustible utilisée dans leurs modèles spécifiques de réaction. Le code neutronique d'EDF COCCINELLE, par exemple, utilise la formule de Rowland, qui emploie les températures de centre et de surface de pastille données.

COCCINELLE est couplé au code thermohydraulique 3D THYC, qui calcule TDoppler grâce à son modèle thermique standard. Pour améliorer la précision de ces calculs, nous avons développé le couplage de nos deux plus récents codes de thermohydraulique (THYC) et de thermomécanique (CYRANO3).

THYC calcule les écoulements diphasiques dans les tuyauteries ou les faisceaux de tubes, et il sert aux calculs de transitoires tels que rupture de la tuyauterie vapeur, accidents de dilution de bore, prédictions de DNB ou études de générateurs de vapeur et de condenseurs.

CYRANO calcule la plupart des phénomènes qui se déroulent dans le combustible : 1) transfert thermique induit par la puissance nucléaire, 2) dilatation thermique du combustible et du gainage, 3) dégagement de produits de fission gazeux, 4) interactions mécaniques entre pastilles et gaines.

Ces deux codes sont désormais qualifiés dans leur domaine respectif, et le couplage, réalisé à l'aide de bibliothèques de machines virtuelles parallèles (PVM), personnalisées sous la forme d'un logiciel développé en interne et d'utilisation facile appelé CALCIUM, a été validé sur des configurations "simples" (pas de dilatation thermique, caractéristiques thermiques constantes), et utilisé sur des transitoires accidentels tels qu'éjection de barre ou perte de refroidissement.

Grâce au couplage déjà existant entre COCCINELLE et THYC, nous serons en mesure, dans un proche avenir, de prendre en compte en neutronique des calculs précis du profil de température du combustible qui conduiront à une approche par meilleure estimation de l'effet Doppler.

EXECUTIVE SUMMARY :

EDF, as the French utility, is responsible for fifty-four. That means numerous calculations of neutronic behaviour have to be carried out for safety in standard or incidental operation, as well as prospective calculations in severe accidents analysis.

Among all parameters, the fuel temperature has a significant influence on the reactivity of the core, because of the Doppler effect on cross-sections.
Most neutronic codes use a straightforward method to calculate an average fuel temperature used in their specific feed-back models. For instance, EDF's neutronic code COCCINELLE uses the Rowland's formula using the temperatures of the center and the surface of the pellet.

COCCINELLE is coupled to the 3D thermal-hydraulic code THYC with calculates TDoppler with is standard thermal model. In order to improve the accuracy of such calculations, we have developed the coupling of our two latest codes in thermal-hydraulics (THYC) and thermo-mechanics (CYRANO3).

THYC calculates two-phase flows in pipes or rod bundles and is used for transient calculations such as steam-line break, boron dilution accidents, DNB predictions, steam generator and condenser studies.

CYRANO3 calculates most of the phenomena that take place in the fuel such as : 1) heat transfer induced by nuclear power ; 2) thermal expansion of the fuel and the cladding ; 3) release of gazeous fission's products ; 4) mechanical interaction between the pellet and the cladding.

These two codes are now qualified in their own field and the coupling, using Parallel Virtual Machine (PVM) libraries customized in an home-made-easy-to-use package called CALCIUM, has been validated on "low" configurations (no thermal expansion, constant thermal characteristics) and used on accidental transients such as rod ejection ~~and loss of coolant accident.~~

Because of the previously existing coupling between COCCINELLE and THYC, we shall be able in a close future to take into account accurate calculations of the fuel temperature profile in neutronics that will lead to a best-estimate approach of the Doppler effect.

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A NEW COUPLING OF THE 3D THERMAL-HYDRAULIC CODE THYC AND THE THERMOMECHANICAL CODE CYRANO3 FOR PWR CALCULATIONS

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I. INTRODUCTION

Because reactor physics is a multidisciplinary approach based upon numerous basic physics such as neutronics, thermal-hydraulics, thermo-mechanics, chemistry and fuel cycle physics, we are faced to an increasing need of coupling specific codes in order to improve "best-estimate" calculations.

The desire to keep each code down to a human scale, essentially in terms of openness and maintenance, means the emphasis is whenever possible given to external coupling of the codes, which then remain independent but communicating computer processes.

For this purpose, EDF has developed in 1993 a general coupler tool called CALCIUM.[1] This home-made tool is now used in most of the coupling made by EDF like COCCINELLE (neutronics)/THYC (thermal-hydraulics)/ CATHARE (global plant operating)[2] and the now presented THYC/CYRANO3 (thermo-mechanics) coupling.

II. THYC: A 3D CODE FOR TWO-PHASE THERMAL-HYDRAULICS FLOW IN BUNDLES[3]

A. General description

Developed at EDF/DER since 1987, THYC calculates one or two phase flows in heated bundles. More intensively qualified on PWR's configuration,[4][5] THYC is mainly dedicated to rod or tube bundles as seen in nuclear cores, steam generators, and condensers.

The physical model used in THYC is composed of three partial differential equations for the mixture of liquid and gas (mass, momentum and energy), one conservation equation for the vapor mass (to treat the subcooled boiling), and one equation on liquid/vapor phase drift velocity.[6] The less present phase is supposed to be at saturation so the sixth equation is not used.

An equivalent porosity ε, which stands for the volume fraction occupied by the fluid, is calculated at the begin of each THYC calculations.

B. Thermal aspects of THYC

There are two different ways of heating the fluid in THYC:

a) No thermal coupling with heating rods. This means that the power is delivered inside the control volume (solids + fluid). The power source in $W.m^{-3}$ is user-given and the flow takes into account the tubes bundle but is not influenced by the thermal properties of rods and cladding.

b) Thermal coupling with heating rods. In this case, the heating flux is given by:

$$\Phi = h^1_{conv}\left(T_{wall} - T_f\right) + h^2_{conv}\left(T_{wall} - T_{sat}\right) \qquad (2)$$

where h^1_{conv} is the correlation-given convective coefficient between the cladding wall and liquid phase; h^2_{conv} is the correlation-given convective coefficient between the cladding wall and the saturated phase.

The power source q is located in the fuel rod and THYC solves the standard heat equation, using a radial nodalization (subscript: m for radial, k for axial) and time:

$$\rho_{fuel}\, C_{P_{fuel}}\, V_m \frac{\delta T_{k,m}}{\Delta t} = \Phi^{t+\Delta t}_{m-1,m}\, S_{m-1,m} - \Phi^{t+\Delta t}_{m,m+1}\, S_{m,m+1} + q^{t+\Delta t}_{k,m}\, V_m \qquad (3)$$

III. CYRANO3: A 2D CODE FOR THERMO-MECHANICS CALCULA-TION OF FUEL ROD

A. General description

CYRANO3 is the brand-new software developed by the Research and Development division for simulation of the fuel rod thermo-mechanical behaviour in order to meet new EDF simulation requirements concerning the fuel, as follows:

1) to raise the combustion rate up to 60,000 MWd/t, that means a better knowledge of high Burn-Up fuel behaviour;

2) to recycle reprocessed Plutonium and Uranium, that means taking into account the thermal / mechanical / chemical proper-ties of the fresh fuel;

3) to introduce burnable poison such as Gadolinium for High Burn-Up purpose, that means a better understanding of the effects of Gadolinium into the UO_2 matrix;

4) to diversify the fuel procurement and to extend the operating specifications, that means an improved control of the design margins;

5) to guarantee the cladding integrity in standard and incidental operating process, that means a good prediction of the chemistry, oxidation, hydridation, and creeping of the Zircaloy cladding.

Developed under strict Quality Assurance rules, it includes three user levels:

1) a designer level with standard fixed options;

2) a R&D level with pluggable functionalities or models;

3) a developer level with easy access to the basic algorithms.

CYRANO3 takes into account:

1) stationary and unstationary modelization of the heat equation in axisymetric geometry;

2) an up-to-date home-made correlation of the fuel thermal conductivity, best-fitted for high burn-up and Gadolinium content;

3) the radialy and axially deformation of the geometry due to thermal expansion and mechanical interaction (fuel-cladding), including the Diabolo effect;

4) the release of gaseous Fission Products;

5) the oxidation/hydridation of the cladding;

6) the fragmentation of the fuel pellet.

B. Thermal-hydraulics aspects of CYRANO3

The default thermal-hydraulics in CYRANO 3 is a conventional monodimensional enthalpy elevation model :

$$\frac{dh}{dt} + u\frac{dh}{dz} = \frac{2\pi R_{wall}\Phi}{\rho_f S_f} \quad (4)$$

Enthalpy is calculated for each time step and axial node. The heat exchange is modeled by the Dittus-Boelter correlation for forced convection, the Jens and Lotte correlation for nucleate boiling and a specific generalized boiling-correlation.

IV. THE CALCIUM COUPLING TOOL[1]

A. General description

CALCIUM is an EDF-made package specialized for building complex coupled systems in FORTRAN language.

Based upon the public domain PVM software (Parallel Virtual Machine) from Oak Ridge National Laboratory, CALCIUM is made of three components: 1) a separate process called the monitor; 2) a library linked to each coupled code; 3) a set of commands designed by the user and specific to the coupling.

The monitor is a kind of data manager where all variables shared by more than one code should be stored.

The possibility of variable interpolation in time is of great interest when time steps are not identical in the coupled codes. This occurs when the physical phenomena don't have the same time scale in each of the codes.

B. Practical use of CALCIUM

Let us illustrate the use of CALCIUM:

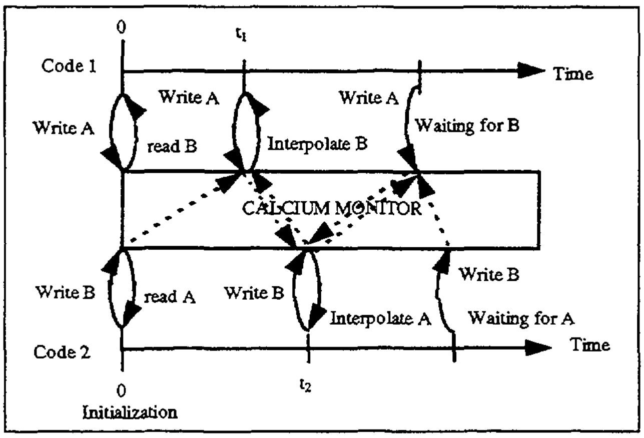

Figure 1: Coupling with CALCIUM

In this case, the code 1 calculates the variable A with an external evaluation of variable B as code 2 calculates B with the help of A. The first step is to initialize the monitor data base with the initial values of A and B then each code can calculate either A^{t_1} or B^{t_2}. If we suppose codes 1 and 2 make real time calculations, code 1 will write A^{t_1} first and wait to interpolate B^{t_1}.

This can be done only when code 2 has calculated B^{t_2} and has written its value in the data base. So code 1 can go on and code 2 must wait for A^{t_2}, and so on for the next time step.

V. THE THYC/CYRANO3 (T/C3) COUPLING

A. Logic of process exchanges (fig. 2)

The transferred variables are given at the frontier of the hydraulics domain, that means the wall of the cladding where CYRANO3 calculates the heat flux : Φ_{wall} through the cladding to the water and THYC calculates in return the temperature of the wall: T_{wall}.

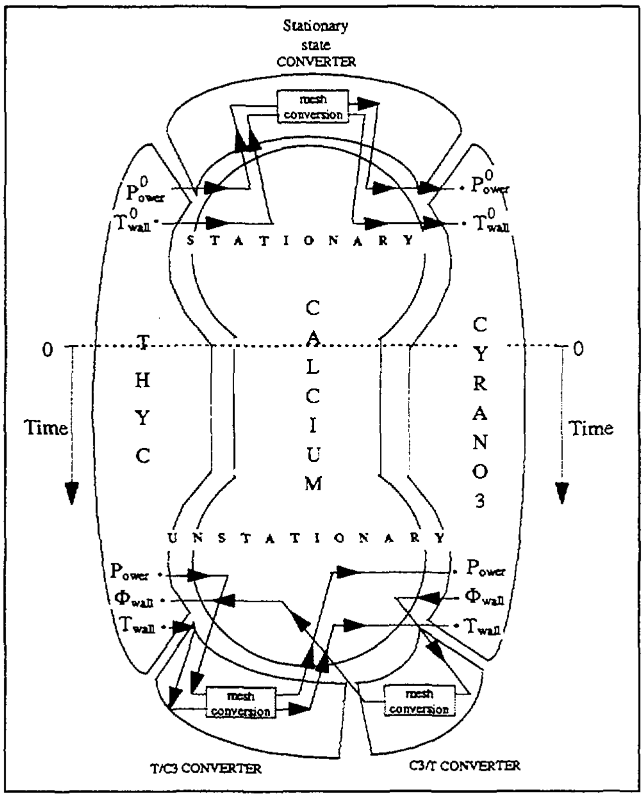

Figure 2: Logic diagram exchanged variables in the coupling THYC/CYRANO3

We have chosen the nuclear power to be transferred by THYC to CYRANO3 because of a future introduction in the existing COCCINELLE/THYC coupling[7] (where COCCINELLE gives the power to THYC, which returns the temperatures of water and fuel rod).

To avoid unnecessary calculations of fuel temperature in THYC during the T/C3 coupling, we use the non-thermal coupling option of THYC previously described and transform the heat flux given by CYRANO3 into a fluid located power source.

B. Need of a mesh converter

Because of different nodalizations of temperature field (fig. 3), we have written a general mesh converter that can interpolate any data field from one nodalization to the other.

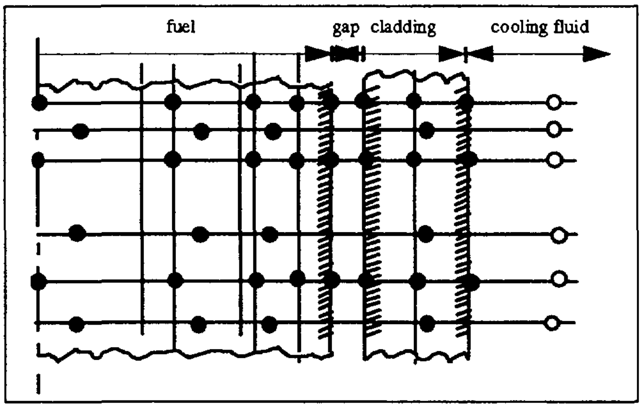

Figure 3: Different nodalization in

THYC ● fuel temperature localization
○ fluid temperature localization

CYRANO3 ● fuel temperature localization
○ fluid temperature localization

We will emphasize the fact that the fuel temperature is no longer needed by THYC in the T/C3 coupling but for upstreaming information to COCCINELLE.

C. Three converters to avoid deadlocks

One can ask what is the need of three separate converters when at first sight one seems enough?

The logic diagram of one converter is the following (fig. 4):

Step CO_1:
Read Power(t) from THYC
Conversion of Power on CYRANO3 nodalization
Send converted Power to CYRANO3

Step CO_2:
Read F(t) from CYRANO3
Conversion of heat flux on THYC nodalization
Send converted heat flux to THYC

Step CO_3:
Read Twall(t) from THYC
Conversion of wall temperature on CYRANO3 nodalization
Send converted Twall(t) to CYRANO3

Figure 4: Logic diagram of one converter

This has to be connected with the THYC and CYRANO3 logic diagrams (fig. 5 and fig. 6).

Step T1: **Send $P_{ower}(t + \Delta t)$**
Step T2: **Read $\Phi(t)$**
Step T3: **THYC calculates**
Step T4: **Send $T_{wall}(t + \Delta t)$**

Figure 5: THYC logic diagram

Step CY_1: **Read $P_{ower}(t)$**
Step CY_2: **Read $T_{wall}(t)$**
Step CY_3: **CYRANO3 calculates**
Step CY_4: **Send $\Phi(t + \Delta t)$**

Figure 6: CYRANO logic diagram

This leads to a dead lock in case of different time steps as illustrated on the snapshot (fig. 7) where steps should be read according to fig. 4, 5 and 6:

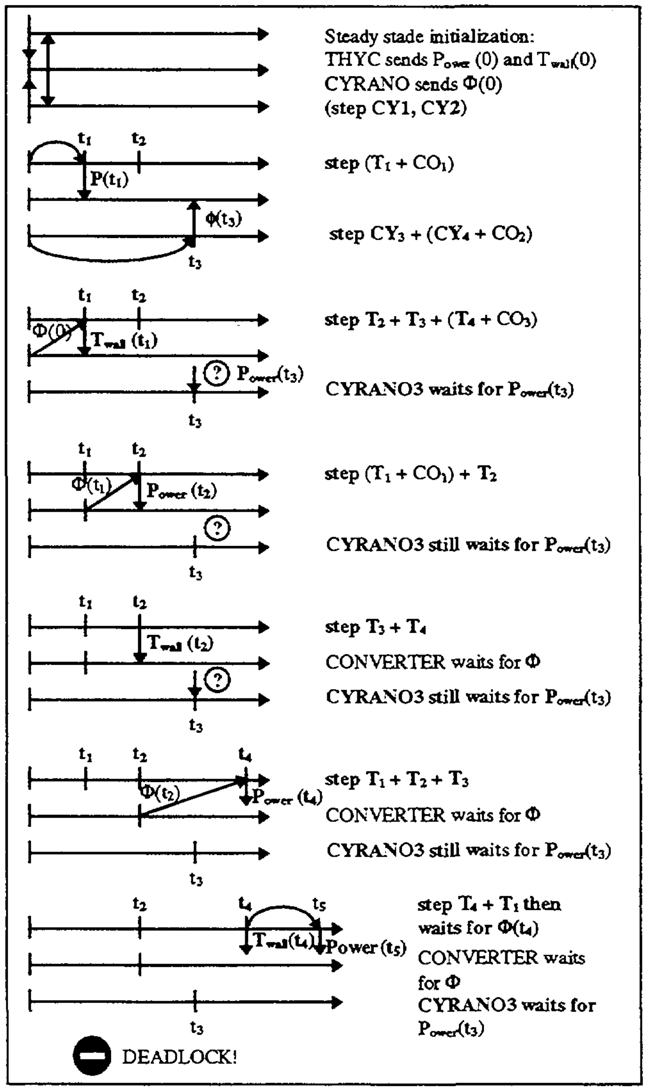

Figure 7: Deadlock using only one converter

The solution consists in three separate converters (fig. 8):

1) one for the stationary state that transfers the targeted power and temperature of the cladding surface from THYC to CYRANO3;

2) two "single-way" converters for unstationary state : the T/C3 converter that transfers as soon as read the Power and T_{wall} and the C3/T for the treatment of Φ_{wall} (fig. 9 and 10).

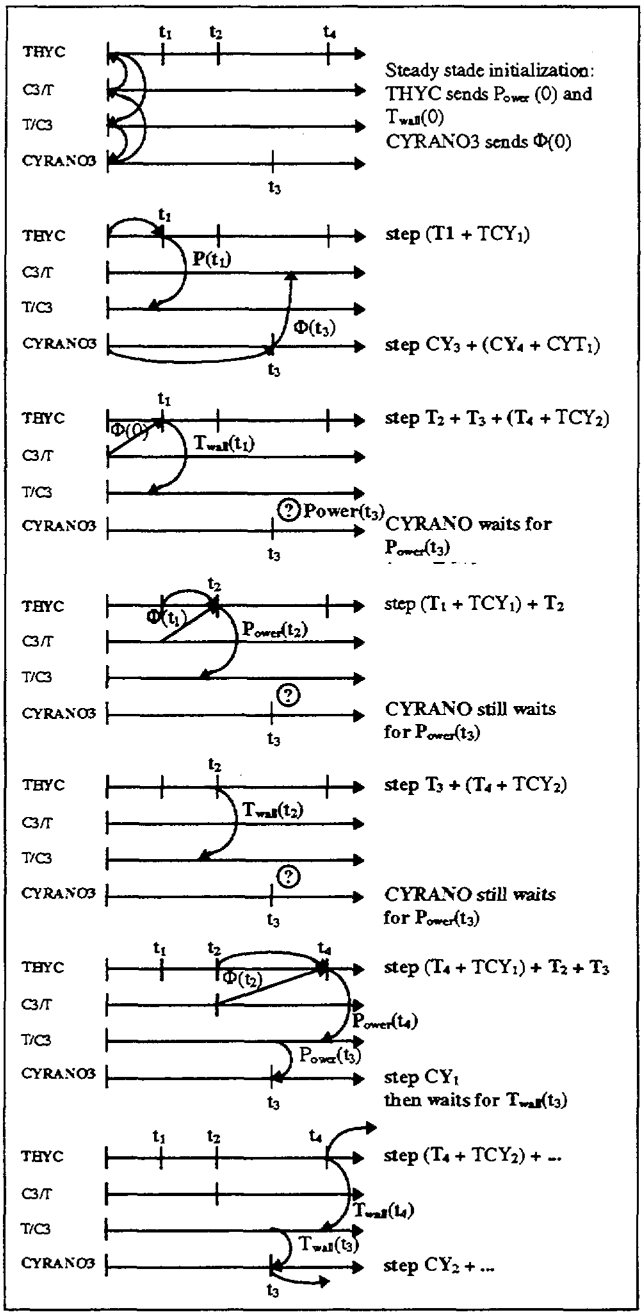

Figure 8: Timing of the T/C3 coupling with two unstationary converters

Step TCY_1:
Read $P_{ower}(t)$ from THYC
Conversion of P_{ower} on CYRANO3 nodalization
Send converted P_{ower} to CYRANO3
Step TCY_2:
Read $T_{wall}(t)$ from THYC
Conversion of wall temperature on CYRANO3 nodalization
Send converted $T_{wall}(t)$ to CYRANO3

Figure 9: THYC to CYRANO3 converter (T/C3)

Step CYT_1:
Read $\Phi(t)$ from CYRANO3
Conversion of heat flux on THYC nodalization
Send converted heat flux to THYC

Figure 10: CYRANO3 to THYC converter (C3/T)

VI. APPLICATION TO A ONE-ROD TRANSIENT CALCULATION

After an extensive phase of qualification, which consists of a comparison between a standard THYC calculation with its own thermal subroutines and a so-called "low configuration" of the T/C3 coupling (that means usual correlations of $\rho \cdot C_p$, λ, h_{gap} and no mechanical deformation are taken into account).

The "full configuration" consists of up-to-date correlation of $\rho \cdot C_p$ and λ, radiative and conductive calculation of h_{gap} and on-line thermo-mechanics and viscoplasticity. We also take into account the feed-back of thermal expansion on hydraulics (because of the change of hydraulic and thermal diameter). This was tested successfully on a SLB power transient (fig. 11) calculated by the neutronic code COCCINELLE:

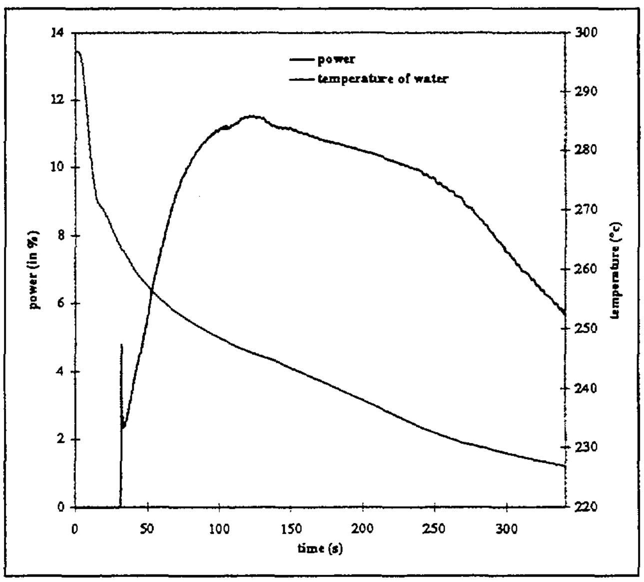

Figure 11: SLB power transient

Tiny differences were obtained on the fuel temperature (fig. 12):

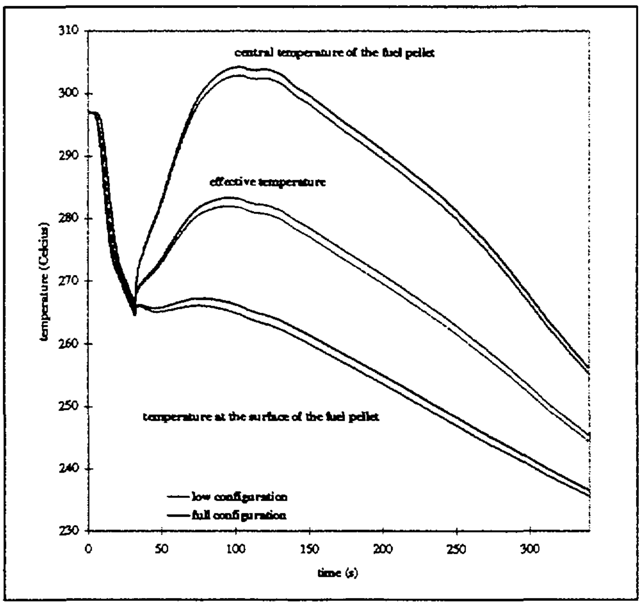

Figure 12: Fuel temperature profile

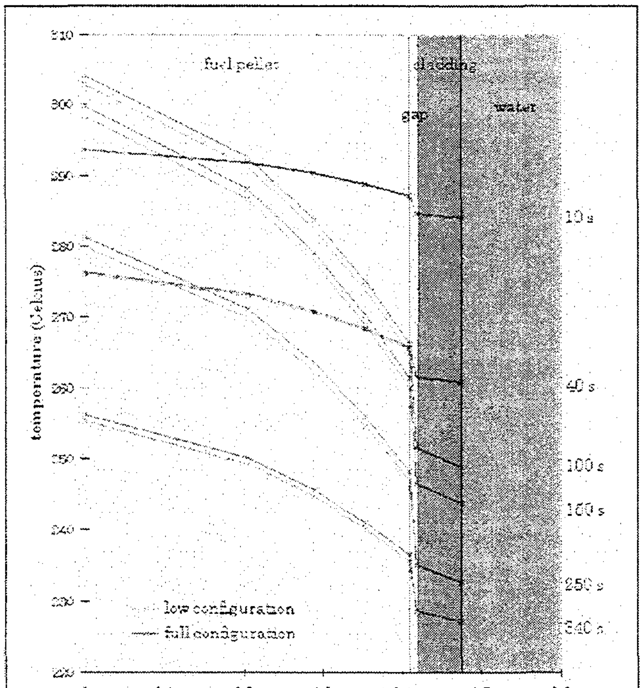

Figure 13: SLB scenario:
Discrepancies of the Doppler effective temperature

Another scenario of rod ejection transient (fig. 14) was chosen because of the high temperature reached.

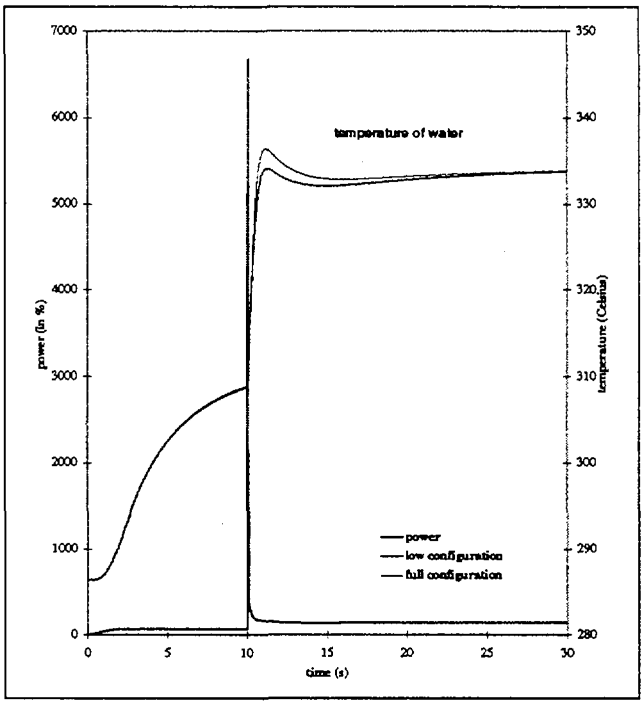

Figure 14: Rod ejection power transient

The pulse of power induces a sudden increase of the fuel temperature, causing the pellet expansion and the gap transfer coefficient increase, as shown, on figure 15:

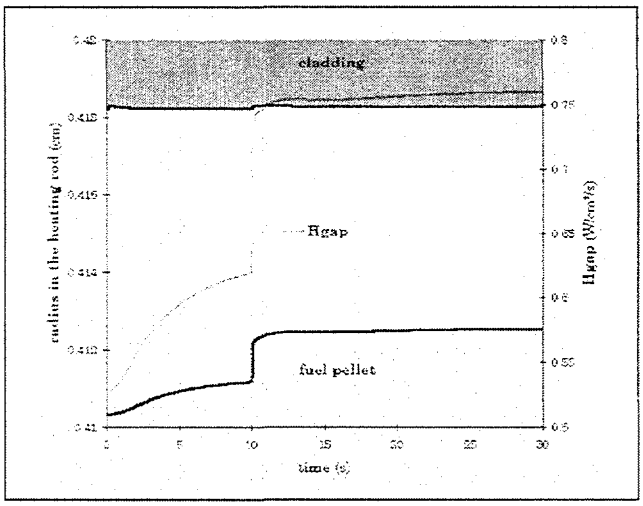

Figure 15: Heat transfer in the gap

Results (fig. 16) show that low configuration over-estimate the Doppler effective temperature by more than 50°C at the end of the scenario. This will have an obvious effect on long term neutronic behaviour.

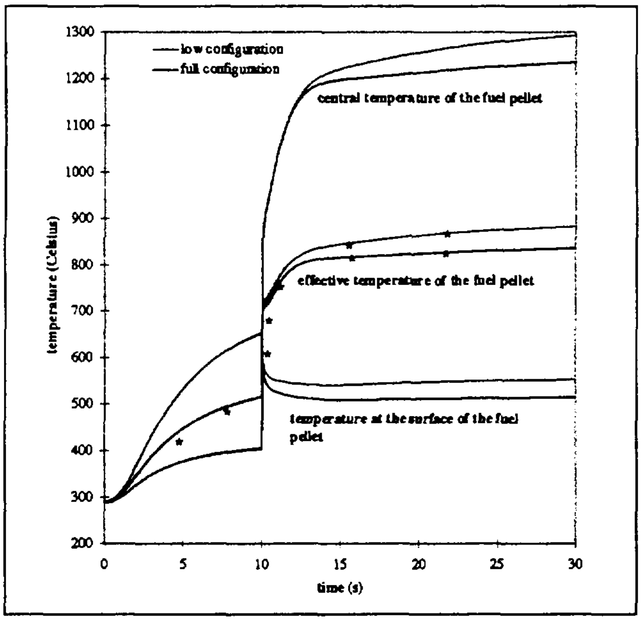

Figure 16: Rod ejection: Discrepancies on the Doppler effective temperature

VII. CONCLUSION

For the first time, as far as we know, an intimate coupling of thermal-hydraulics and thermo-mechanics has been realized for neutronic purpose. Effects can be huge depending on the scenario.

Further parametric studies will determine the effects of high burn-up. But the next big step is to introduce the feed-back of this newly calculated Doppler effective temperature on cross-sections. This will be obtained by the coupling of COCCINELLE/THYC/CYRANO3, then the power transient will be affected by the best-estimate fuel temperature, a milestone for accidental core calculations.

VIII. NOMENCLATURE

C_p	thermal capacity
h	fluid enthalpy
h_{conv}	convection transfer coefficient
q	power density
R_{wall}	external radius of the cladding
S_f	surface of the flow
$S_{m,m+1}$	surface between pellet node m and m + 1
t	time
T	temperature
u	mixture velocity
V_m	volume of the pellet node m
Φ	heat flux
λ	thermal conductivity
ρ	density

Subscripts

f	fluid
k	axial node
m	radial pellet node
wall	cladding wall
sat	saturation

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