

# **A PIN-BY-PIN FUEL TEMPERATURE MODEL FOR LWR DETAILED NEUTRON KINETICS AND THERMAL HYDRAULICS CALCULATIONS**

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## **ABSTRACT**

The pin-by-pin model based on the advanced heterogeneous reactor theory was developed in RRC “Kurchatov Institute” for analysis of light water reactor (LWR) transients including reactivity initiated accidents (RIAs). This model implemented in the BARS neutronic code was validated against various numerical and experimental benchmarks. A coupling of the BARS code with the RELAP5/MOD3.2 thermal-hydraulic code is used for VVER and PWR rod ejection accident (REA) analysis. In practice of calculations, RELAP could not be used for full-scale pin-by-pin core thermal-hydraulic analysis because of input deck restrictions and extremely large running time. To extent capabilities of such an analysis, a pin-by-pin fuel temperature model has been developed and incorporated into the RELAP-BARS coupled code. This model is based on a reconstruction method for a pin-by-pin fuel temperature distribution within each fuel assembly using a simple analytical procedure. To validate the pin-by-pin fuel temperature model and to access intra-assembly effects due to non-uniform fuel temperature distribution within the assembly, a control rod ejection accident in the TMI-1 PWR with a high burnup fuel core has been calculated by the RELAP-BARS code. Validation results for the reconstruction method compared with the RELAP “direct” calculation showed that the pin-by-pin model for fuel temperature is quite adequate: uncertainty in the fuel temperature increment for the hottest fuel pellet does not exceed 1.5%. A comparison of the calculational results obtained by using the assembly averaged and pin-by-pin models for the fuel temperature distribution within the reactor core, showed that the deviation in local fuel enthalpy increment for the hottest fuel rod does not exceed 2% during the transient.

# 1. INTRODUCTION

In some RIAs in LWRs, such as ejection of a peripheral control rod, steam line break or boron dilution, large deformations in the power distribution over the reactor core can occur during the transient. A key factor in safety analysis of RIA consequences is peak local fuel enthalpy used as the acceptance criterion of fuel pin integrity, especially in a case of RIAs in a LWR with a high burnup core. The RIA calculational analysis is carried out by widely spread 3D assembly-by-assembly neutron kinetics codes coupled with modern thermal-hydraulic codes such as TRAC, RELAP5, and etc. These neutronic codes, which are known as “best-estimate”, are based, as a rule, on a two-group nodal diffusion model. They calculate assembly average power distribution during the transient and thermal-hydraulic calculations are based solely on these data. Thus, estimation of the peak local fuel enthalpy may be done only by using additional procedure of a power reconstruction within the fuel assembly containing the hottest fuel pin. Usually, such a procedure is used only for the assembly with peak power. But, as it was shown in reference 1, the hottest fuel pin does not necessarily belong to the hottest fuel assembly. Another problem deals with reliability of a power reconstruction model under the transient conditions, especially, for an assembly located near the core reflector. (It is worth to note that enthalpy is an integral parameter and in case of very large deformations in the power distribution during the transient, calculation of local fuel enthalpy will require rather complicated procedure to take into account such effects.)

A pin-by-pin model allows to take into account the intra-assembly effects directly without any additional procedure of the power reconstruction. Such a detailed NPP dynamic model has been developed in Russian Research Centre “Kurchatov Institute” for VVER and PWR RIA calculations. The model is based on coupling of the RELAP5/MOD3.2 thermal hydraulic code with the BARS neutronic code.<sup>2-4</sup> The 3D pin-by-pin heterogeneous model (up to 80,000 pins) describes core neutronics, but thermal hydraulic processes in the core are described by multi-channel assembly-by-assembly model. An individual thermal hydraulic channel corresponds to each fuel assembly and only few hot fuel rods are simulated by individual thermal structures. Validation calculations carried out for various numerical and experimental benchmarks<sup>4-6</sup> show that the BARS code meets accuracy criteria for LWR RIA analysis and coupled RELAP-BARS code can be successfully used for RIA modeling.

By now, a pin-by-pin fuel temperature model has been developed and incorporated into the NPP dynamic model. It should be noted that in practice the RELAP code could not be used for full-scale pin-by-pin core thermal hydraulic calculations because of input deck restrictions and extremely large running time. That is why a new method to reconstruct 3D pin-by-pin fuel temperature distribution has been developed.

Section 2 focuses on features of the heterogeneous method. Section 3 contains description of the RELAP-BARS coupled model for LWR RIA analysis. Section 4 presents the reconstruction method for the pin-by-pin fuel temperature representation. Section 5 assesses the effects of the pin-by-pin fuel temperature representation on consequences of the TMI-1 PWR REA.

## 2. ADVANCED HETEROGENEOUS METHOD

The BARS code was developed on the basis of the advanced method of heterogeneous reactor theory. The method is based on analytical representation of the neutron flux distribution as a superposition of Green's functions. In LWR applications this method allows directly to take into account complicated core geometry by explicit representation of fuel pins, absorber rods, etc. Green's function is derived from a solution of few group diffusion equations in an infinite uniform media with a singular source at the cell axis. The intensities of the singular sources are determined in such a way that relationship between neutron flux and current at the boundary of each reactor cell coincides with that obtained from the precise transport calculation for a single cell. The latter relationship is defined by means of a boundary condition matrix ( $\Lambda$ -matrix). This matrix is determined from neutron transport calculations of the cell with varying neutron currents at the its boundary.<sup>7</sup>

An axial distribution of the neutron flux is described by Fourier series expansion. As a result, it is derived a set of linear algebraic equations which establish a relationship between any pair of the reactor cells. It leads to unresolved computation problem in reactor calculations: only a core with few cells could be calculated by using even modern computers. To transform these equations to connect only neighboring cells, a difference approximation of Green's functions is performed.<sup>8</sup>

To calculate fast transients, the heterogeneous method uses "time absorption" matrices instead of the traditional neutron velocities.<sup>3</sup> Within any time step a spatial-time neutron flux distribution is represented as a product of a time-dependent amplitude function and a spatial-dependent form-function (quasi-static approach). The amplitude function is determined as a solution of point kinetic equations. Parameters of these equations are calculated by a perturbation theory method. The form-function is determined by solving a system of linear equations with a delayed neutron source. To reduce the number of 3D calculations during the RIA, a term describing the reactivity dependence due to reactor energy release feedback is included into the point kinetic equations.

It should be noted that the heterogeneous theory does not require the validity of the diffusion approximation over the reactor. The diffusion equations are used only to determine Green's function shape that weakly influences the reactor calculation accuracy. It is very important for a pin-by-pin calculation of LWRs containing modern fuel assemblies with heterogeneous structure. Note that unlike a homogenized calculation, a pin-by-pin one requires a rather large number of energy groups because of a small size of cells. As the BARS validation results showed,  $\Lambda$ -matrix approach allows to do LWR pin-by-pin calculations with reasonable accuracy using 4-5 groups.

The BARS neutron database ( $\Lambda$ -matrices) is prepared by the TRIFON code,<sup>7</sup> which solves the multigroup neutron transport equation for various reactor cells using the collision probability method taking into account detailed structure of resonant cross sections. Strong resonances are calculated explicitly using fine energy mesh within the resonance and weak resonances are taken into account using an effective resonance level model.<sup>9</sup> This allows to reduce total number of groups up to about 350. The TRIFON neutron database is generated on the basis of ENDF/B-VI library by the NJOY code.<sup>10,11</sup>

### 3. DESCRIPTION OF THE RELAP5-BARS COUPLED MODEL

In LWR analysis an important feature of the RELAP-BARS coupled code is a relatively large running time for a single calculation by BARS in comparison with RELAP. The quasi-static approach used in the BARS kinetic model allows to choose time step for reactor calculation depending only on degree of relative variations in the power distribution shape, in spite of the fact that the total reactor power and thermal hydraulic parameters may varied. In virtue of it, the BARS time step, as a rule, is much larger than the RELAP one, except for time periods with fast insertion of the reactivity in the core (for instance, a control rod ejection).

For this reason, the neutronic calculation in each time step is divided into the following stages:

1. Calculation of the neutron flux form-function and the delayed neutron precursor distribution. This requires the largest computational time.
2. Calculation of the point kinetic parameters, the amplitude function and determination of the pin-by-pin power distribution. This requires a much smaller computational time compared with a single RELAP calculation.

At the first stage calculations are performed rather seldom and depend on changes in the reactor power distribution. At the second stage calculations are carried out at each RELAP time step.

In the framework of the RELAP model, the BARS neutronic calculation can be considered as determination of the core power distribution as a function of time and spatial coordinates for the RELAP next time step taking into account thermal hydraulic feedbacks. In this case the BARS code can be treated as a subroutine of the RELAP code.

To provide the data exchange between RELAP and BARS, the COTT interface code is used. This code calculates also pin-by-pin fuel temperature distribution by the reconstruction method and some additional thermal hydraulic parameters, which are not calculated by RELAP. Besides, the COTT code contains simplified thermal hydraulic option based on 1D single- or two-phase homogeneous flow with a slip ration. This option is used for thermal-hydraulic calculation of the core during slow transients such as, for example, fuel burnup (fuel cycle modeling).

Before the transient modeling, the RELAP-BARS code calculates the initial steady state. The neutronic calculation is performed by the BARS steady-state option, which solves the non-linear eigenvalue problem. During the coupled neutronic – thermal-hydraulic calculation the core initial conditions can be automatically adjusted.

The following possibilities are available for the adjustment in the BARS code:

- change in the neutron generation rate,
- change in the axial position of some control rods or control rod banks,
- change in the boric acid concentration in the coolant.

Then the dynamic calculation is performed: the neutronic calculation is carried out by the BARS time-dependent option and the thermal-hydraulic calculation - by the RELAP dynamic option. Figure 1 shows the scheme of the RELAP-BARS coupled calculations.

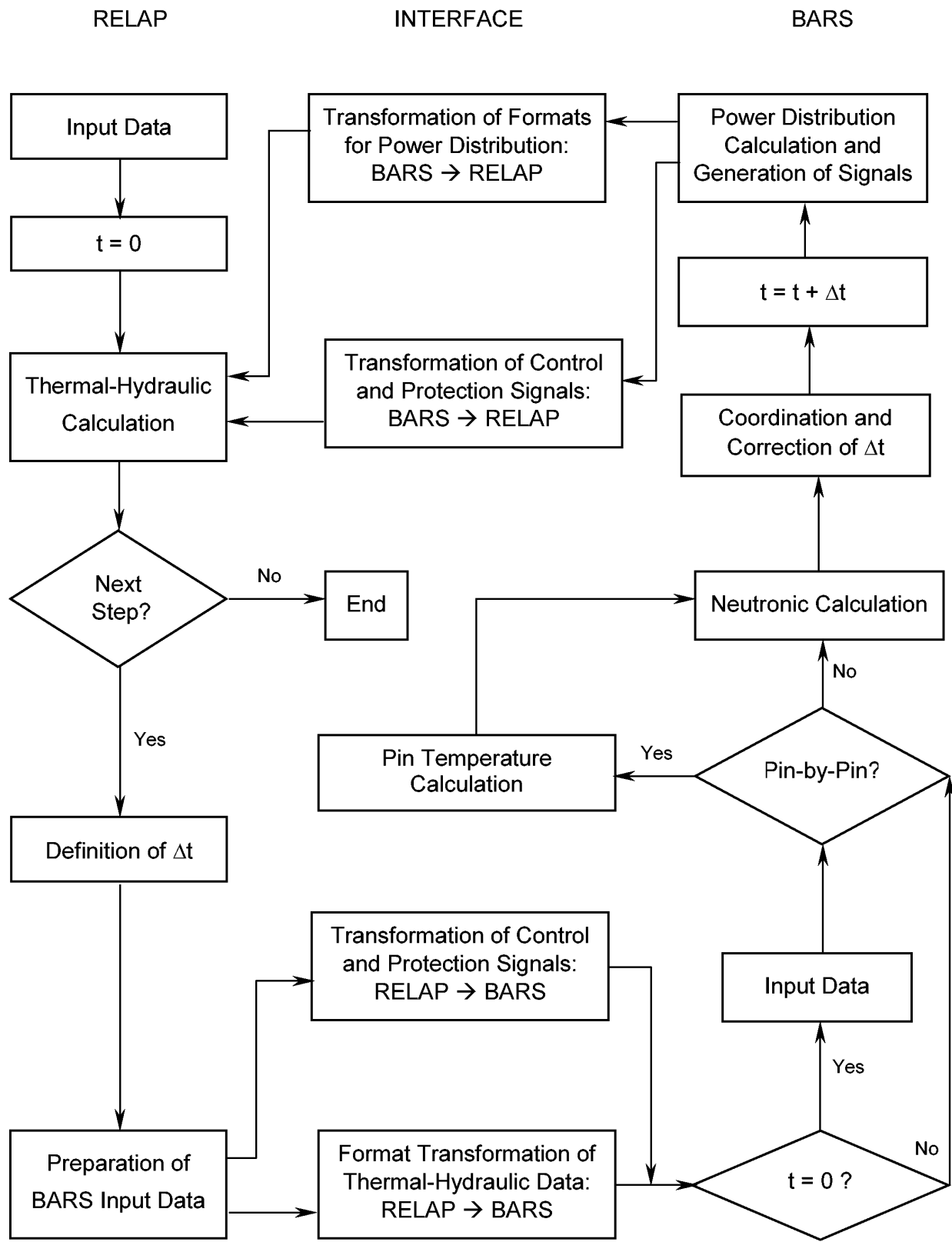


Figure 1. Scheme of the RELAP-BARS Coupling.

#### 4. RECONSTRUCTION OF THE PIN-BY-PIN FUEL TEMPERATURE DISTRIBUTION

In practice of calculations, the RELAP code could not be used for full-scale pin-by-pin core thermal-hydraulic analysis because of input deck restrictions and extremely large running time. That is why a new method to reconstruct a 3D pin-by-pin fuel temperature distribution within any fuel assembly was developed. Since a few hottest fuel pins can be calculated by RELAP directly, the fuel temperature reconstruction is needed mainly to take into account the effect of the intra-assembly fuel temperature distribution on the Doppler feedback. This effect is not expected to be large, so a very high accuracy in the pin-by-pin fuel temperature reconstruction is not required. From the other side, such a procedure has to be fast-running, because of total number of the fuel pins in LWR cores is typically about 50,000. Taking into considerations all these circumstances, it was developed the reconstruction method based on a simple analytical procedure.

The proposed method uses a representation of the radial averaged fuel rod temperature in any axial node as a sum of two terms. If  $T(t)$  is the radial averaged fuel temperature calculated by RELAP for the rod with average power in given axial layer, then “reconstructed” averaged temperature in any fuel rod with index “k” at the same axial layer  $T_k(t)$  is defined as:

$$T_k(t) = T(t) + \theta_k(t) \quad (1)$$

where

$t$  is the time,

$\theta_k(t)$  is the temperature deviation.

To obtain the expression for  $\theta_k(t)$ , the following approximations are used:

- the heat transfer coefficient, the coolant temperature, and the fuel and cladding volumetric heat capacities and conductivities are identical for all fuel rods within the assembly,
- the fuel thermal conductivity and volumetric heat capacity are determined by  $T(t)$ ,
- a radial dependence of  $\theta_k$  is described by a parabola;
- a radial dependence of the deviation of the cladding temperature from the cladding temperature for the rod with averaged power is linear.

Within any RELAP time step these approximations allow to formulate the linear Fourier equations for the radial dependence of the fuel and cladding temperature deviations. Integrating and summing these equations over the radial direction, the heat balance equation for the rod is obtained. It contains a heat flux at the cladding surface. To exclude the heat flux from the heat balance equation, the boundary condition at the cladding surface and the approximations for the fuel and cladding temperature deviations are used. As a result the following equation for  $\theta_k(t)$  is derived:

$$c \frac{d\theta_k(t)}{dt} = q_k(t) - \frac{2}{r} \alpha \theta_k(t), \quad t_{j-1} \leq t \leq t_j \quad (2)$$

with the initial condition at time moment  $t_0$ :

$$\theta_k(t_0) = \theta_k^0 \quad (3)$$

and

$$q_k(t) = Q_k(t) - Q(t), \quad (4)$$

$$\frac{1}{\alpha} = \frac{1}{\alpha_f} + \frac{1}{\alpha_g} + \frac{1}{\alpha_c} + \frac{1}{\alpha_\ell} \quad (5)$$

where

- $c$  is the fuel volumetric heat capacity,
- $Q_k(t)$  is the fuel rod volumetric heat source, calculated by BARS,
- $Q(t)$  is the assembly average volumetric heat source,
- $r$  is the fuel pellet radius,
- $j$  is the RELAP time step index,
- $\alpha_f$  is the fuel thermal conductivity,
- $\alpha_g$  is the gas gap thermal conductivity,
- $\alpha_c$  is the cladding thermal conductivity,
- $\alpha_\ell$  is the cladding-coolant thermal conductivity.

The differential equation (2) has a simple analytical solution that can be written for any RELAP time step with index “ $j$ ” as below:

$$\theta_k(t_j) = \frac{q_k(t_j)}{\alpha} \left[ 1 - \exp\left(-\frac{\alpha}{c\Delta t_j}\right) + \theta_k(t_{j-1}) \cdot \exp\left(-\frac{\alpha}{c\Delta t_j}\right) \right], \quad \Delta t_j = t_j - t_{j-1} \quad (6)$$

Thus, the determination of the pin-by-pin fuel temperature distribution consists of two stages:

- an assembly-by-assembly fuel temperature calculation by the RELAP code using an assembly averaged power distribution, calculated by the BARS code;
- pin-by-pin fuel temperature reconstruction within each assembly by the COTT code used as an interface code between RELAP and BARS.

## 5. CALCULATION OF PWR REA

This Section describes RELAP-BARS calculational efforts aimed to understand the uncertainty in analysis of effects of the detailed intra-assembly fuel temperature representation on neutronic and thermal-hydraulic parameters during a PWR REA. These calculations were done as part of a joint NRC–IPSN–RRC KI study<sup>12</sup> to understand the uncertainty in best-estimate calculations of the local fuel enthalpy during such a transient.

The analysis of intra-assembly effects due to fuel temperature representation was made using two different approaches in the calculation of the fuel temperature: assembly-by-assembly (Case 1) and pin-by-pin (Case 2). The last model is based on the fuel temperature reconstruction method described in previous section. In both models the same pin-by-pin power calculational approach is used. The major difference between two models was the representation of the fuel temperature within any assembly. In Case 1 the single axial distribution of the fuel temperature of the pin with averaged power was used for all pins within the assembly. While in Case 2 each fuel pin has its own axial fuel temperature distribution calculated using the corresponding power distribution.

The reactor model used in the RELAP-BARS calculations was based on the PWR of Three Mile Island Unit 1 that was chosen as an international benchmark.<sup>13</sup> The reactor core with one-eight symmetry contains 177 fuel assemblies with fuel burnup ranged from 23 up to 58 GWd/t (the end of the cycle). The BARS neutron database was generated using data on fuel nuclide compositions averaged over each assembly in each axial layer were used. This information was received from U.S. partners. Thus, fuel pins within each assembly in each axial layer had the same set of  $\Lambda$ -matrices. There were totally 24 axial layers for the active part of the core, which contains 36,816 fuel pins. The total number of calculational nodes in the reactor model was about 1,000,000.

Initial conditions were hot zero power (HZP) with 20 control rods of 3 regulating banks fully inserted in the core as shown on Figure 2. As a basis scenario, an ejection of central rod H8 with an ejection time of 0.1 s was chosen. The figure indicates that all inserted control rods are located at assemblies with high burnup fuel. It is obvious that after withdrawal of one of them, peak power will be observed in any neighboring assembly having relatively low burnup. In case of withdrawal of rod H8, power reaches its peak value in assembly H9, which does not contains any control rods and has average burnup of 30 GWd/t. Figure 3 shows layout of a fuel assembly. It should be noted that assembly H9 contains also two hottest pins located near the water gap between both assemblies as shown on Figure 3.

HZP conditions (the fuel and coolant temperature at 551K) are characterized rather significant axial peaking factor in the neutron flux of about 3 with shifting of the maximum to the top part of the core. Due to such an axial non-uniformity, it is necessary to use no less than 20 harmonics in the BARS calculations. All the calculations were performed using 4 energy groups for prompt neutrons and 6 groups for delayed neutrons. The value of the delayed neutron fraction ( $\beta$ ) was 521 pcm.



	8	9	10	11	12	13	14	15
H	52.86 Bank 7	30.19	56.25	30.85	49.53 Bank 7	28.11	53.86 Bank 6	55.78
K		57.94	30.80	55.43	29.83	53.95 Bank 5	25.55	49.17
L			57.57 Bank 6	30.22	54.40	27.86	23.30	47.30
M				49.71 Bank 5	28.85	52.85	40.94	
N					48.75 Bank 7	23.86	41.45	
O						37.34		

52.86	- fuel burnup (GWd/t)
Bank 7	- No. of regulating Bank

Figure 2. One-Eight Core Layout.

Before REA modeling, a number of steady-state calculations were carried out using RELAP-BARS coupled code. As a result of these calculations, there were defined some neutronic and thermal-hydraulic parameters (worth of the ejected control rod and regulating banks, the Doppler and moderator temperature coefficients of reactivity) which could effect on consequences of the REA. Table I summarizes the basic steady state parameters.

Table I. Steady-State Parameters.

Parameter	Value
Worth of Bank 5 (pcm)	1548
Worth of Bank 6 (pcm)	859
Worth of Bank 7 (pcm)	1105
Worth of rod H8 (pcm)	338
Worth of rod H12 (pcm)	202
Worth of rod N12 (pcm)	543
Doppler coefficient (pcm)	-2.8
Isothermal temperature coefficient (pcm/K)	-46.8

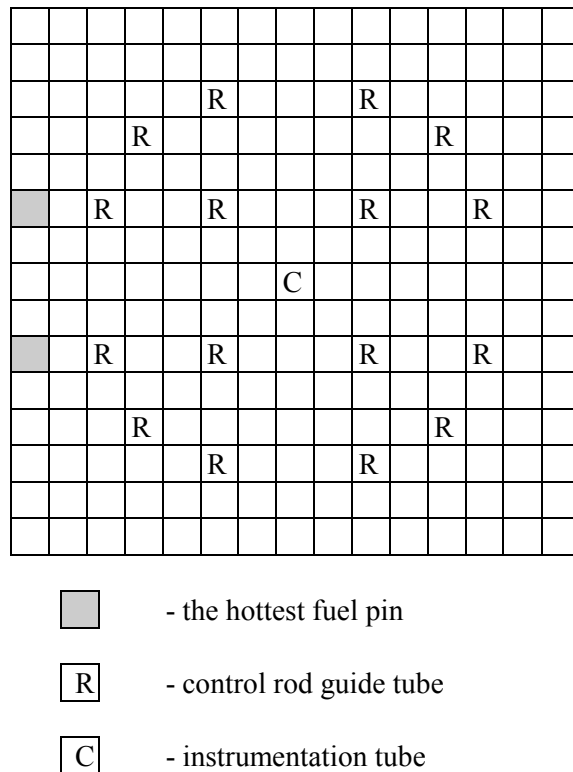


Figure 3. Layout of a Fuel Assembly.

The steady state results show that the worth of control rod H8 (considered as the ejected one) is only about  $0.65\beta$ . It is clear that such a REA is characterized a power excursion below prompt-critical. Consequently, this would not result in fuel damage in no case. To provide conservative conditions of the REA the worth of the ejected rod was artificially increased up to  $1.2\beta$ . Duration of the process was chosen as 2.5 s; no scram was assumed during the transient.

The validation of the reconstruction method for the intra-assembly fuel temperature distribution within any assembly was done directly during the REA calculation. For this reason some fuel pins of interest were considered as separate heat structures in the RELAP input deck. It allowed comparing fuel temperatures in selected fuel pins calculated “directly” by the RELAP code and by “approximate” reconstruction method.

Figure 4 shows fuel temperature increment for the hottest fuel pellet calculated “directly” (solid curve) and relative deviation between “approximate” and “direct” calculations (dashed curve) as a function of the time of the transient. As it was shown in the figure, the relative uncertainty of the reconstruction method for the hottest fuel pin compared with the “direct” calculation did not exceed 1.5% during the transient (this resulted in the temperature deviation of no more than 1.5K at the time of the peak power). Thus, the following conclusion can be done: the reconstruction method allows to calculate the fuel temperature distribution within any assembly during a REA with a reasonable accuracy.

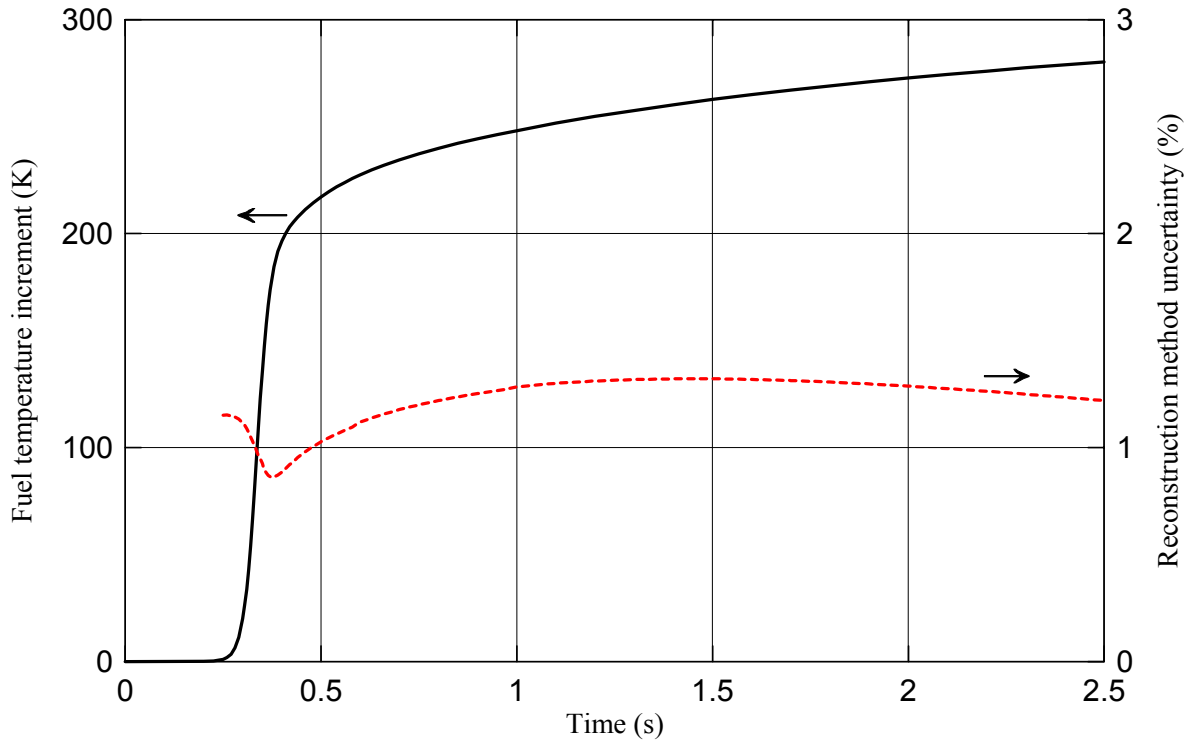


Figure 4. Fuel Temperature Increment in the Hottest Fuel Pellet vs. Time.

Table II presents major parameters of the transient calculated by both models: the assembly-by-assembly (Case 1) and pin-by-pin fuel temperature representation (Case 2). The last column gives relative deviation between Case 2 and Case 1.

Table II. Main Parameters of the REA with Different Fuel Temperature Models.

Parameter of transient	Case 1	Case 2	Deviation
Control rod worth ( $\beta$ )	1.209	1.209	-
Peak power of the core (GW)	10.69	10.51	-1.7%
Time of peak power (ms)	338	338	-
Power pulse width (ms)	63.0	63.0	-
Peak power of the fuel pin (kW)	835	821	-1.7%
Maximum increment in fuel enthalpy (cal/g)	20.6	20.3	-1.4%

Figures 5 and 6 show reactor power and enthalpy increment for the hottest fuel pellet as functions of the time of the transient. These dependencies are given as solid curves calculated for Case 2. Here the relative deviations between Case 2 and Case 1 are indicated as dashed curves. As the figures show, the relative difference in calculations of the reactor power and the fuel enthalpy obtained by two methods did not exceed 2.5% with decreasing to 1% at the end of the transient.

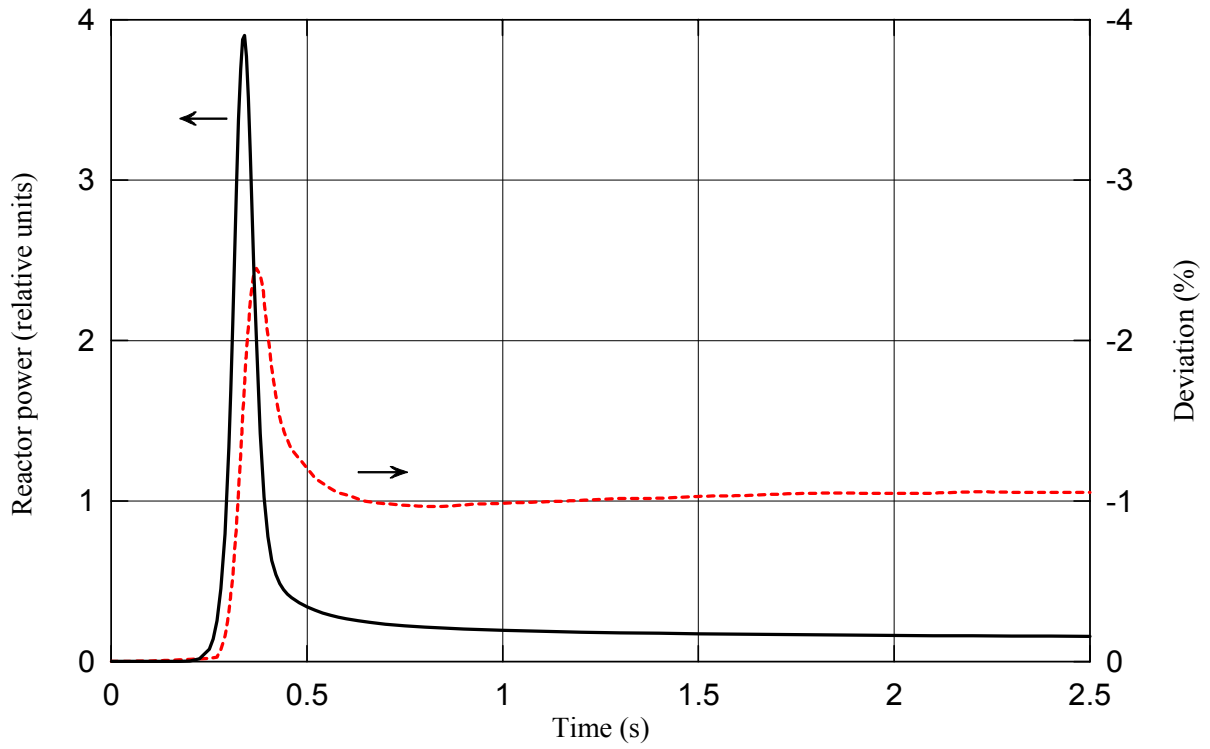


Figure 5. Reactor Power vs. Time.

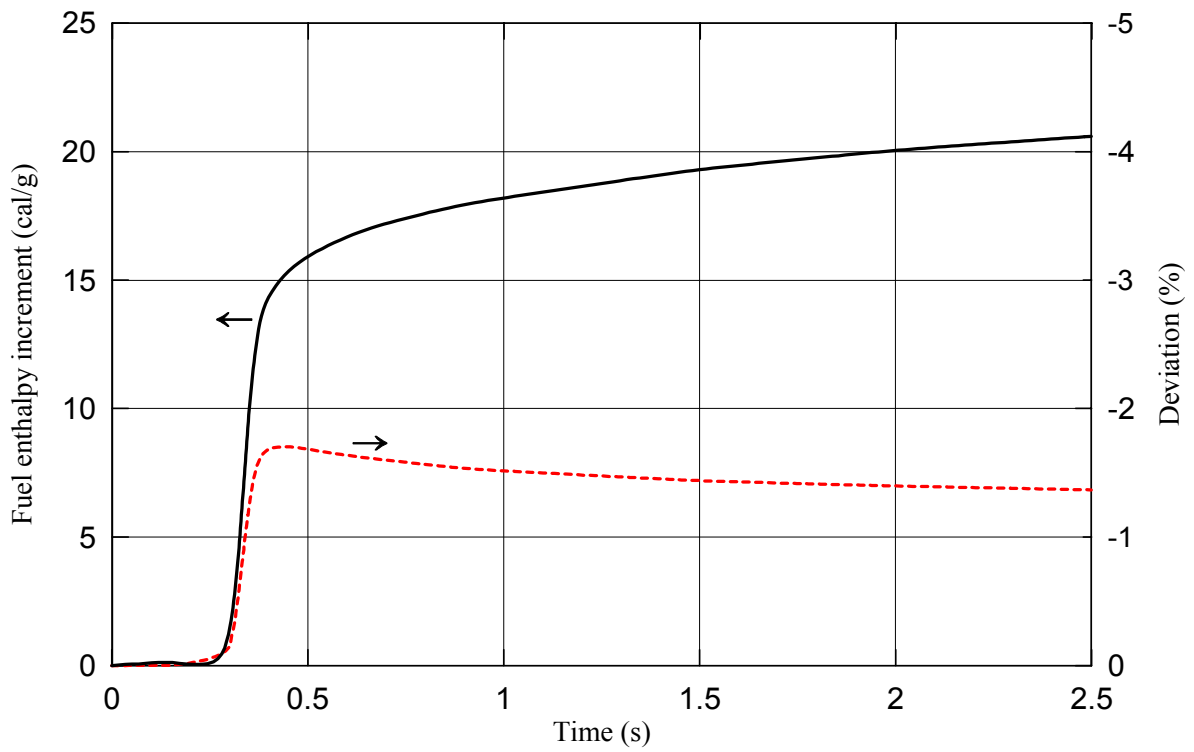


Figure 6. Enthalpy Increment for the Hottest Fuel Pellet vs. Time.

As Figure 5 shows, the reactor power reaches its peak at 0.34 s when the maximum increase in fuel temperature for the hottest pellet in assembly H9 was about 100K (see Figure 4). At the same time the maximum difference in fuel temperature for the hottest layer in this assembly was about 10K. Such relatively low fuel temperature non-uniformity and not great fuel temperature increment during the transient were key factors which allow to understand why all parameters calculated in both cases are well agreed.

At the end of the transient the maximum increase in fuel temperature for the hottest pellet in reached 283K and the maximum difference in fuel temperature across the assembly became 33K as can seen on Figure 7. As the calculational results shown, the last parameter did not exceed 70K in any axial layer of any fuel assembly.

831	823	820	820	820	820	820	816	816	816	812	808	805	801	801
827	816	812	816	820	823	816	808	812	820	808	805	797	797	801
831	816	816	823	827		820	808	816		820	812	801	797	801
831	820	823		831	823	812	805	812	820	823		812	801	805
834	823	831	831	827	827	816	808	812	820	820	820	816	808	808
834	831		827	827		823	816	823		820	816		812	808
834	823	823	816	816	827	827	834	827	820	812	808	812	808	808
834	820	812	812	812	820	834		834	812	805	801	801	801	808
834	823	823	816	816	827	827	834	827	820	812	808	812	808	808
834	831		827	827		823	816	823		820	816		812	808
834	823	827	831	823	823	812	805	808	820	816	820	816	805	808
831	816	823		827	823	812	805	808	816	820		808	797	805
831	812	812	820	823		816	805	812		816	808	797	793	801
827	816	812	812	816	820	812	805	808	816	808	801	797	793	801
831	823	820	820	820	820	820	816	816	816	812	808	805	801	801

Figure 7. Fuel Temperature Distribution for the Hottest Layer in Assembly H9.

Comparison of the presented results shown that calculation with assembly-by-assembly fuel temperature representation gave slightly conservative results in key parameters of the considered REA compared with the pin-by-pin one.

It should be mentioned that in such a transient with ejection of the central control rod it was not observed significant deformations in the power distribution over the core. For this reason the maximum fuel temperature and enthalpy increment are far less than the acceptance criteria. In case of ejection of the peripheral control rod N12 (see Figure 2), large deformations in the power distribution occur. Moreover, as the calculations shown, such an accident would be more realistic because the required value of the inserted reactivity (more than  $1\beta$ ) is may be realized under the assumption of stuck rod M11. In this case the intra-assembly effects due to fuel temperature representation are expected to be larger.

## CONCLUSIONS

This study was performed with aim to understand the uncertainty in calculation of major safety parameters of the PWR REA due to different models of the fuel temperature representation. The analysis was done for the central rod ejection accident in the TMI-1 PWR with a high burnup fuel core. All calculations were carried out using the RELAP-BARS coupled code in which the BARS neutronic model is based on the pin-by-pin approach, while the thermal-hydraulic RELAP model uses assembly-by-assembly approach.

To extent capabilities of the RIA analysis, the pin-by-pin fuel temperature model has been developed. This model is based on the reconstruction method for a pin-by-pin fuel temperature distribution within each fuel assembly. Validation of the method carried out as part of the REA calculation confirmed its reliability: uncertainty in the fuel temperature increment for the hottest fuel pellet did not exceed 1.5%.

The comparison of the calculational results obtained by using the assembly averaged and pin-by-pin models for the fuel temperature distribution within the reactor core, showed that the deviation in local fuel enthalpy increment for the hottest fuel rod did not exceed 2% during the transient. The assembly-by-assembly fuel temperature representation gave slightly conservative results in the REA key parameters (such as local fuel enthalpy) compared with the pin-by-pin one.

## ACKNOWLEDGEMENTS

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