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VERIFICATION OF J-TRAC CODE WITH 3D NEUTRON KINETICS MODEL SKETCH-N FOR PWR ROD EJECTION ANALYSIS

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KEY WORDS

Three-dimensional neutron kinetics, TRAC code, coupling, PVM, NEACRP PWR rod ejection benchmark.

ABSTRACT

A three-dimensional neutron kinetics model is implemented into the transient reactor analysis code J-TRAC to improve the best-estimate analysis of the events requiring multidimensional core modeling. The neutronics model is the SKETCH-N code, which can solve a steady-state, adjoint and kinetics form of neutron diffusion equations in X-Y-Z geometry. The efficient polynomial and semi-analytic nodal methods based on the nonlinear iteration procedure are used in the code. A consistent mapping procedure is developed to perform the data exchange between the TRAC code, which considers the reactor vessel in R-θ-Z geometry and the SKETCH-N code, which applies X-Y-Z spatial mesh. The data transfer is implemented using the message-passing library Parallel Virtual Machine (PVM) providing a portability of the coupled code for different computer platforms. A verification of the J-TRAC/SKETCH-N code system is performed against the PWR rod ejection benchmark. A comparison of the results with the reference solution demonstrates a good accuracy in the parameters important for the rod ejection analysis: time and value of the power peak and maximum fuel centerline temperature.

1. INTRODUCTION

Rod ejection accidents (REA) remain an important aspect of the Pressurized Water Reactor (PWR) safety. A rapid ejection of the control rod assembly from a PWR

core can happen due to a mechanical failure of the control rod housing. In the case of hot zero power conditions, the consequence of this failure is a super-prompt-critical reactivity insertion, which results in a fast core power excursion terminated by the Doppler feedback. The codes based on the point kinetics models traditionally have been used for the REA analyses (Diamond, 1987). However, utilization of the high burn-up fuel, which undergoes cladding failure at significantly lower deposited energy than the current safety limits (Fuketa et al., 1996) renews an interest in the REA analysis using more accurate models. 3D neutron kinetics codes have been recently applied for the both best-estimate and conservative analysis (for example, K. Ivanov et al., 1997). There are several reactor analysis code systems, like ANC/VIPRE (Chao and Sung, 1998), PANBOX (Boer et al., 1992) etc., which can be used for such purposes. The system transient analysis codes, which recently implemented 3D neutron kinetics models, for example, ATHLET code coupled with several neutron kinetics codes (Langenbuch et. al, 1996), RELAP5/NESTLE (Judd et al., 1994), RETRAN-3D/ARROTTA (Goose et al., 1998), TRAC-PF1/NEM (Bandini, 1998) can be also applied. PWR rod ejection benchmark (Finneman and Galati, 1992) was carried out by Nuclear Energy Agency through its Reactor Physics Committee (NEACRP) to give the first survey of the state of the art in this area. The benchmark has been extensively used to verify coupled neutronics/thermal-hydraulics code systems; the first results of the benchmark participants are published in the benchmark report (Finneman et al., 1993).

This paper describes a coupling of the transient analysis code J-TRAC with the 3D neutron kinetics code SKETCH-N and presents the code system verification for the REA analysis by the NEACRP PWR rod ejection benchmark.

2. J-TRAC CODE

J-TRAC code (Akimoto et al., 1989) is the best-estimate two-fluid thermal-hydraulic code TRAC-PF1/Mod1 (Lilies et al., 1988) modified in JAERI to improve the simulation of reflooding phenomena during loss-of-coolant accidents. The verification of the reflooding model of the J-TRAC code is given in (Akimoto et. al., 1988), summary of the TRAC-PF1/MOD1 assessment results is presented in (Sahota and Addessio, 1985).

The J-TRAC code has models of major PWR components: ACCUMULATOR, PRESSURIZER, PUMP, STEAM GENERATOR, TURBINE, VESSEL et al. Using these components and control system, a code user can simulate many PWR transients. The reactor core is modeled by the VESSEL component, which solves six two-phase flow fluid dynamics equations in R-θ-Z geometry, heat conduction equations in the fuel rods and point kinetics equations to calculate the power distribution. The point kinetics model significantly limits the best-estimate capabilities of the J-TRAC code for many PWR transients. To remove this limitation a coupling with the 3D neutron kinetics code SKETCH-N has been performed.

3. SKETCH-N CODE

The SKETCH-N code (Zimin and Ninokata, 1998) solves neutron diffusion equations in X-Y-Z geometry for steady-state, adjoint and neutron kinetics problems. The code can treat an arbitrary number of neutron energy groups and delayed neutron

precursors. The efficient polynomial and semi-analytic nodal methods based on the nonlinear iteration procedure can be used for spatial discretization of diffusion equations (Zimin et al., 1998). Time integration of the neutron kinetics problem is performed by the fully implicit scheme with an analytical treatment of the delayed neutron precursors. Steady-state eigenvalue problems are solved by inverse iterations with a Wielandt shift, the Chebyshev adaptive iterative procedure is used for the neutron kinetics problems. The block symmetric successive overrelaxation method (SSOR) is applied as a preconditioner in the both iterative procedures. Automatic time step control procedure based on the time step doubling technique is used in the code.

An extensive set of the steady-state and neutron kinetics Light Water Reactor (LWR) benchmarks has been calculated to verify the SKETCH-N code. The steady-state problems include: the classical 2D & 3D International Atomic Energy Agency PWR problems; 2D Biblis PWR checker-board-loaded core; 2D Zion-1 PWR problem with explicit modeling of the baffle; 2D 4-group Koeberg PWR checker-board-loaded core with realistic cross sections including up-scattering (Zimin et al., 1998). The neutron kinetics module has been verified against 3D Langenbuch-Maurer-Werner (LMW) operational transient in a small PWR model; and 2D & 3D super-prompt-critical rod drop accident in Boiling Water Reactor (BWR) (Zimin and Ninokata, 1998). The verification results show that the SKETCH-N code has acceptable accuracy and efficiency to be used in the LWR safety analysis and design.

4. COUPLING AND DATA TRANSFER BETWEEN THE CODES

The coupling and data transfer between the codes is organized using the message-passing library Parallel Virtual Machine (PVM) (Al Geist et al., 1994). The codes are treated as separate processes and the subroutines based on PVM are responsible for a data exchange between the codes and a synchronization of time stepping. Flow chart of the coupled J-TRAC/SKETCH-N calculations is illustrated in Fig. 1. After performing an input, the J-TRAC code enrolls into PVM and spawns the child process - SKETCH-N. When SKETCH-N is started, it gets an identification number of the parent process and the codes can communicate to each other sending/receiving messages. At the beginner of a time step, J-TRAC sends a message to SKETCH-N with thermal-hydraulics reactor data (fuel temperature, coolant density and coolant temperature) and an estimation of the next time step size. SKETCH-N receives the message, selects a new time step size and performs the neutronics calculations. Then, SKETCH-N sends a message to J-TRAC with the computed power distribution and the used time step size. J-TRAC receives the message and performs the thermal-hydraulics calculation. The procedure is repeated till the end of the transient.

The J-TRAC code and the SKETCH-N code perform calculations using different spatial meshes and even different coordinate systems. Moreover, the J-TRAC code applies axially different (staggered) meshes for the fluid dynamics model and the heat conduction model. An example of the axial meshes used in the codes is given in Fig. 2.

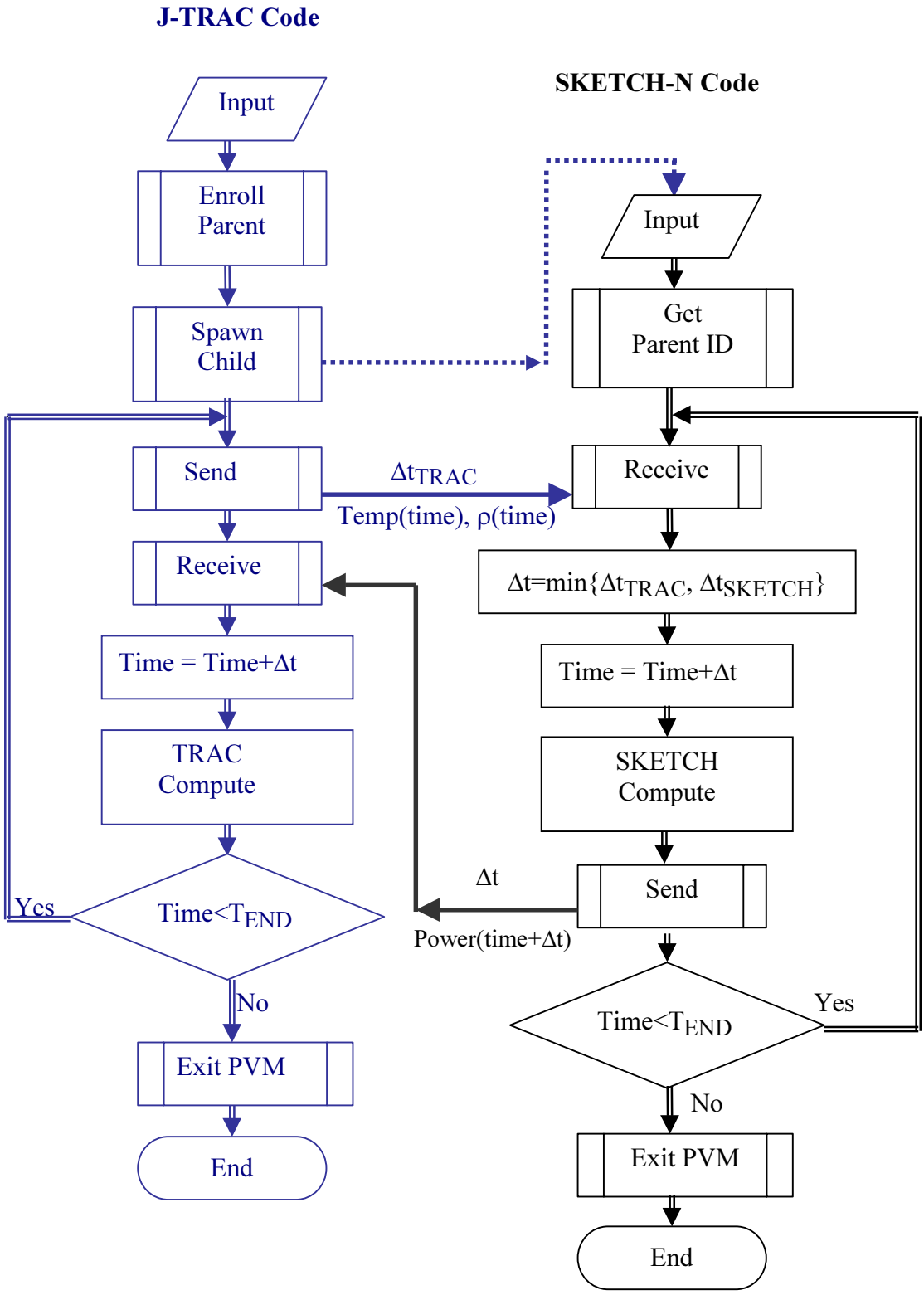

Fig. 1 Simplified flow chart of the J-TRAC/SKETCH-N calculations.

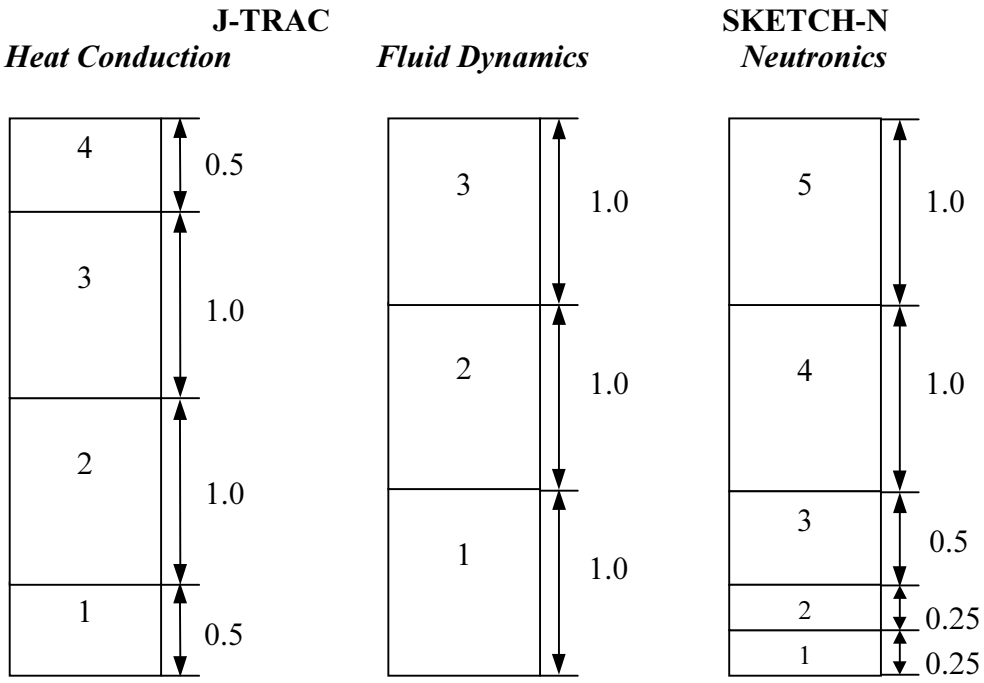

Fig. 2 An example of the axial meshes in the J-TRAC and SKETCH-N codes.

The coupled J-TRAC/SKETCH-N calculations require a mapping of the data between the neutronics, heat conduction and fluid dynamics meshes. The list of the variables, which transfer between the meshes, is given as follows

- from the neutronics mesh into the heat conduction mesh:

  heat generation rate of the heat conduction nodes;

- from the neutronics mesh into the fluid dynamics mesh:

  heat generation rate of the fluid dynamics nodes due to direct coolant heating;

- from the heat conduction mesh into the neutronics mesh:

  average Doppler fuel temperature of the neutronics nodes;

- from the fluid dynamics mesh into the neutronics mesh:

  average coolant temperature and coolant density of the neutronics nodes.

Note that the term “node” is used in the context of a finite-volume method to specify a control volume, not a mesh point.

The mapping procedure between the meshes is based on the mapping matrix approach developed for the PARCS code (Downar et. al, 1997). Let us consider the mapping of the

heat generation rate computed by the SKETCH code on the neutronics spatial mesh into the heat conduction mesh and into the fluid dynamics mesh. The mapping is performed using the two mapping matrices: S^{HC}_{NEUT} and S^{FD}_{NEUT}. Even the spatial meshes of SKETCH-N and J-TRAC codes can be very different they share the one common feature: a 3D spatial mesh of the both codes is a tensor product of the 2D spatial mesh in radial plane and the 1D axial mesh. As a result the 3D mapping matrix can be also expressed as a tensor product of the 2D and 1D mapping matrices:

$$S = S2D \otimes S1D \tag{1}$$

where $\otimes$ is a direct (Kronecker) matrix product; $S2D$ is the mapping matrix describing a correspondence of 2D radial meshes; $S1D$ is the mapping matrix for axial meshes.

These mapping matrices $S2D$ and $S1D$ are defined by a code user for two pairs of the spatial meshes: neutronics mesh $\Rightarrow$ heat conduction mesh and neutronics mesh $\Rightarrow$ fluid dynamics mesh. Let us consider the calculation of the mapping matrix for two 1D axial meshes: the neutronics mesh z with J nodes, *j*-th node is the interval $[z_j, z_{j+1}]$ and the heat conduction mesh Z with I nodes, *i*-th node is the interval $[Z_i, Z_{i+1}]$. The mapping matrix S1D for these two meshes is computed as

$$S1D_{ij} = \frac{\left| [z_j, z_{j+1}] \cap [Z_i, Z_{i+1}] \right|}{\left| [z_j, z_{j+1}] \right|}, \tag{2}$$

where $[z_j, z_{j+1}] \cap [Z_i, Z_{i+1}]$ is an intersection of the intervals $[z_j, z_{j+1}]$ and $[Z_i, Z_{i+1}]$; $|\circ|$ is the function equals to the length of the interval.

For example, the mapping matrices for the axial meshes defined in Fig. 2 are given as

$$S1D^{HC}_{NEUT} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 & 0.5 \\ 0 & 0 & 0 & 0 & 0.5 \end{pmatrix}; \quad S1D^{FD}_{NEUT} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

where $S1D^{HC}_{NEUT}$ is the mapping matrix from the neutronics mesh into the heat conduction mesh; $S1D^{FD}_{NEUT}$ is the mapping matrix from the neutronics mesh into the fluid dynamics mesh.

The calculation of the mapping matrices for 2D spatial meshes is very similar, the only difference that the area of the nodes is taken instead of the length of the nodes. Because the mapping matrices are very sparse, a compressed row storage format is used for their input and storage (Barrett et al., 1994).

According to the definition (see Eq. 2), the mapping matrices satisfy the following condition

$$\sum_{i=1}^{I} S_{ij} = 1$$

This condition providing the conservation law is checked in the code, when the input of the mapping matrices is performed.

Using the defined mapping matrices the heat generation rate on the heat conduction mesh $P\,[HC]$ is computed as

$$P\,[HC] = (\,1-\alpha\,)\; S_{NEUT}^{HC}\; P\,[NEUT]\,,$$

where α is a part of the energy directly deposited into the coolant; $P[NEUT]$ is the heat generation rate computed by the SKETCH-N code on the neutronics spatial mesh; S_{NEUT}^{HC} is the 3D mapping matrix from the neutronics mesh into the heat conduction mesh computed using Eq. (1).

The heat generation rate on the fluid dynamics mesh $P\,[FD]$ is computed as

$$P\,[FD] = \alpha\; S_{NEUT}^{FD}\; P\,[NEUT]\,,$$

where S_{NEUT}^{FD} is the 3D mapping matrix from the neutronics mesh into the fluid dynamics mesh computed using Eq. (1).

The data mapping from the J-TRAC spatial meshes into the neutronics mesh is performed in a similar fashion. The Doppler fuel temperature computed by J-TRAC code on the heat conduction mesh $TF[HC]$ is mapped into the neutronics mesh as

$$TF[NEUT] = S_{HC}^{NEUT}\; TF[HC]\,,$$

where $TF[NEUT]$ is the Doppler fuel temperature on the neutronics mesh, S_{HC}^{NEUT} is the mapping matrix from the heat conduction mesh into the neutronics mesh.

If geometry is specified consistently for the both codes, the mapping matrix S_{HC}^{NEUT} is simply a transpose of the mapping matrix S_{NEUT}^{HC} :

$$S_{HC}^{NEUT} = \left(S_{NEUT}^{HC}\right)^{T}$$

The treatment of the coolant temperature and coolant density is slightly more involved. Due to the donor-cell method used in the J-TRAC code, the computed coolant

temperature and coolant density are the values at the interfaces of the fluid dynamics nodes. To get the node-average values of the coolant temperature on the fluid dynamics axial mesh the linear interpolation is applied as follows

$$TC^{n}[FD] = 0.5\left(TC^{n}[FD\_TRAC] + TC^{nn}[FD\_TRAC] \right),$$

for n = 1, …,N;

where $TC[FD]$ is the node-average value of the coolant temperature; n is an axial index of the node; $TC[FD\_TRAC]$ is the coolant temperature computed by the J-TRAC code; and

$nn = \begin{cases} n-1, & \text{if} \quad V_Z > 0 \\ n+1, & \text{if} \quad V_Z < 0 \end{cases}$; where V_Z is the coolant velocity in axial direction.

The coolant density is interpolated in the same way. Then, the node-averaged values of the coolant density and the coolant temperature are mapped into the neutronics mesh in the similar way as described above for the fuel temperature.

5. NEACRP PWR ROD EJECTION BENCHMARK

The NEACRP PWR rod ejection benchmark was proposed by H. Finnemann and A. Galati (1992) and has been widely used for the verification of coupled neutronics/thermal-hydraulics codes (Finnemann et al., 1993). The PWR core is derived from the real reactor geometry and operational data. The transients are initiated by a rapid ejection of a control rod at the hot zero power (cases A1, B1 and C1) or full power (cases A2, B2 and C2). The reactor geometry has 1/8 core symmetry in the cases A and B and ½ core symmetry in the cases C. The detail benchmark description is given in (Finnemann and Galati, 1992); the paper by Chao and Sung (1998) provides comments on some ambiguities of the benchmark specification. A reference solution of the benchmark is computed by the PANTHER code using fine temporal and spatial meshes (Finnemann et al., 1993). Recently, Knight and Bryce (1997) are published a refined reference solution, where additional sensitivity analysis is performed and uncertainties of the results are significantly decreased.

5.1 SKETCH-N Model

The neutronics model has two neutron energy groups and six groups of delayed neutron precursors. Reactor core is specified at the beginner of Cycle 1. The reactor core configuration for the cases A and B is illustrated in Fig. 3. 11 material compositions are defined to simulate fuel assemblies with the different fuel enrichment and a different number of rods of burnable absorbers. The macro cross sections are given as polynomial functions of the control rod position, boron concentration, effective fuel temperature, coolant density and coolant temperature. The SKETCH-N calculations were performed using a quarter-core representation for the cases A and B and a half-core representation for the cases C. A neutronics spatial mesh was defined with 4 nodes per fuel assembly in

radial plane and 18 axial layers specified in the benchmark. In the initial condition, a reactor is critical and a value of the critical boron concentration should be computed. An automatic time step control procedure based on the time step doubling technique (Zimin and Ninokata, 1998) was used to determine the time step size. A temporal truncation error tolerance was set to 5×10^{-3}. The performed sensitivity study has shown that the given tolerance provides a temporally convergent solution. A one update of the nodal coupling coefficients per time step was used in the nonlinear iteration procedure. The default iterative convergence criteria (10^{-5} for the steady-state problems and 10^{-4} for kinetics problems) were applied.

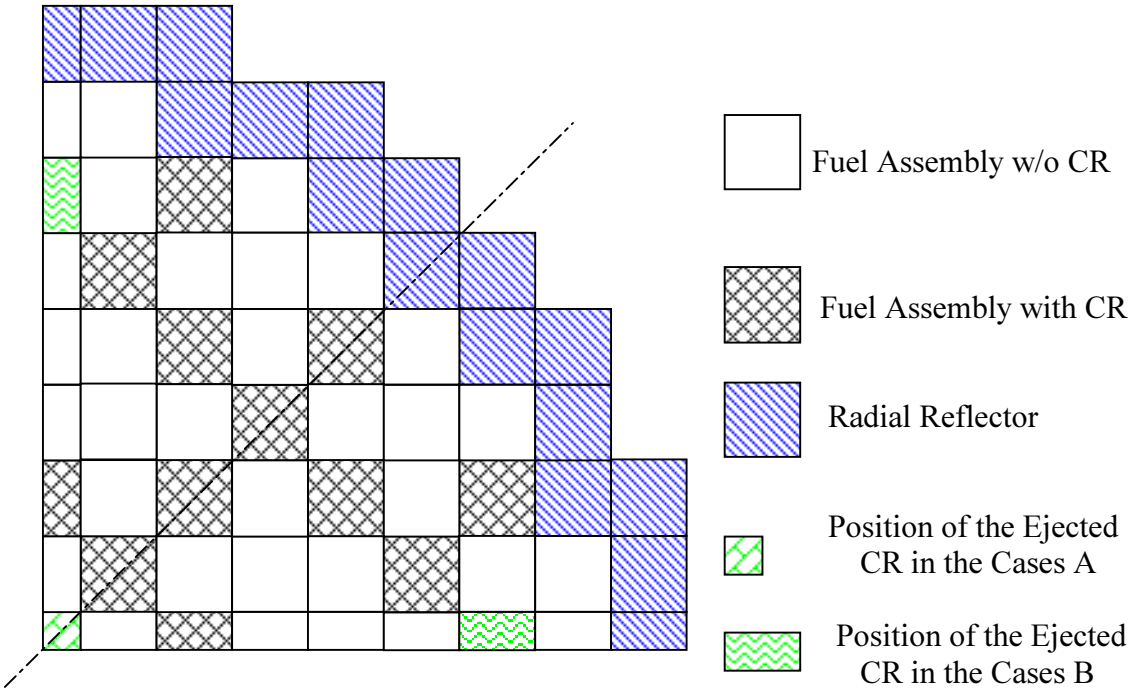

Fig. 3 PWR NEACRP Core Model of the Cases A and B.

5.2 J-TRAC Model

In the J-TRAC code, the VESSEL component is used to simulate the reactor. Spatial mesh in R-θ plane contains 27 nodes (3 rings and 9 sectors) for the cases A and B and 88 nodes (11 rings and 8 sectors) for the cases C. In the cases A and B, each of the 26 nodes simulates a single fuel assembly of the 1/8 core representation and 1 node models a radial reflector. In the cases C, 86 nodes are used for fuel assemblies and 2 nodes for radial reflector. Each of three small axial neutronics layers on the top and on the bottom of the reactor core are combined into the single fluid dynamics layer, the resulting axial spatial mesh has 14 layers. The radial heat conduction mesh has 9 zones in the fuel, 1 in the gap and 2 in the cladding. The reactor boundary conditions are given

using the FILL components on the bottom, which define the mass flow rate and the BREAK components on the top, which specify the reactor pressure. Zero lateral cross flow is simulated setting to zero the cross flow areas in R and θ directions. The material properties defined in the benchmark are implemented as an option in the J-TRAC code. A direct coolant-heating model has been also developed for the VESSEL component of the J-TRAC code.

5.3 Numerical Results

Table 1 represents the steady-state results of the cases A1, B1 and C1 defined at the hot zero power (HZP) and the cases A2, B2, and C2 defined at the full power (FP). In the HZP cases, the J-TRAC/SKETCH-N results are in an excellent agreement with the PANTHER reference solution (Knight and Bryce, 1997), confirming accuracy of the semi-analytic nodal method of the SKETCH-N code. In the case of FP conditions, the J-TRAC/SKETCH-N slightly underestimates the ejected control rod worth and overestimates the power peaking factor; however, the deviations are rather small.

Table 1 The J-TRAC/SKETCH-N steady-state results of the PWR NEACRP rod ejection benchmark (upper values), PANTHER reference solution (middle values) and the deviations from the PANTHER reference solution *(lower values).*

Parameter	Hot Zero Power (HZP)			Full Power (FP)		
	Case A1	Case B1	Case C1	Case A2	Case B2	Case C2
Critical Boron Concentration, ppm	561.9 561.20 *+0.7 ppm*	1248.7 1247.98 *+0.7 ppm*	1129.2 1128.29 *+0.9 ppm*	1155.4 1156.63 *-1.2 ppm*	1182.2 1183.83 *-1.6 ppm*	1155.6 1156.63 *-1 ppm*
3D Nodal Power Peaking Factor	2.8770 2.8792 *-0.08 %*	1.9333 1.9330 *+0.02 %*	2.1873 2.1867 *+0.02 %*	2.2223 2.2073 *+0.7 %*	2.1107 2.0954 *+0.7 %*	2.2213 2.2073 *+0.6 %*
Control Rod Worth, pcm	822.2 824.31 *-2 pcm*	826.4 826.18 *+0.2 pcm*	948.4 949.09 *-0.7 pcm*	85 91.58 *- 7 pcm*	92 99.45 *- 7 pcm*	74 79.23 *-5 pcm*

The transient calculations were performed using the automatic time step control procedure. The selected time step sizes are shown in Fig. 4 for the cases A1 and A2. The total reactor power versus time is given in Fig. 5 and 6 for the HZP and FP cases, respectively. Fig. 7 presents the reactor-averaged Doppler fuel temperature versus time for the HZP cases; Fig. 8 demonstrates the maximum fuel centerline temperature versus time for the same cases. The PANTHER results at the time of power peak (for reactor power) and at the time 5 s (for fuel temperature) are also shown at these figures. It is interesting to note that the average Doppler fuel temperature is the lowest in the Case B1 while the maximum fuel centerline temperature is the highest in the same case. These

results outline an importance of the accurate treatment of the spatial effects in the rod ejection analysis.

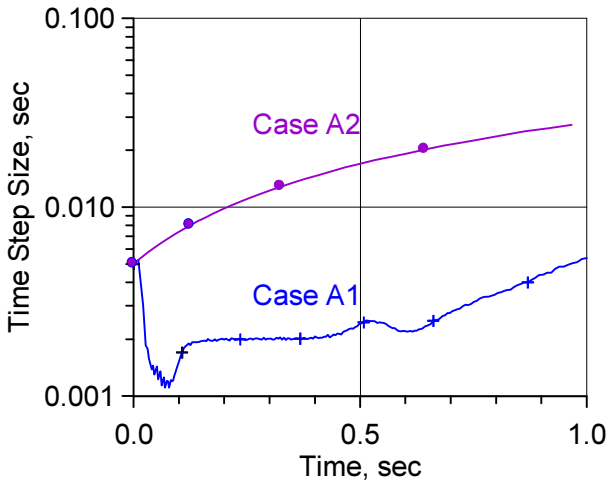

Fig. 4 Selected time step size for the cases A1 and B1.

The summary of the transient results and a comparison with the PANTHER reference solution is given in Table 2. The comparison results show that the coupled J-TRAC/SKETCH-N code system can accurately predict the most important parameters in the rod ejection analysis: the time and value of the power peak and the maximum fuel centerline temperature. The maximum error in the power peak is 3.0 % (case A1); the maximum error in the fuel centerline temperature is 20 °C or 1.2 % (case B2).

Table 2 J-TRAC/SKETCH-N transient results of the PWR NEACRP rod ejection benchmark (upper values), PANTHER reference solution (middle values) and deviations from the PANTHER reference solution *(lower values)*.

Parameter	Hot Zero Power (HZP)			Full Power (FP)		
	Case A1	Case B1	Case C1	Case A2	Case B2	Case C2
Time to the Power Peak, s	0.547 0.5375 *+0.01 s*	0.525 0.5225 *+0.003 s*	0.2732 0.2712 *+0.002* s	0.095 0.095 -	0.095 0.1 *-0.005 s*	0.095 0.095 -
Power at the Peak, %	123.0 126.78 *-3.0 %*	229.7 231.51 *-0.8 %*	437.0 441.12 *-1 %*	108.0 108.3 *-0.3 %*	106.4 106.4 -	107.25 107.34 *+0.1 %*
Power at 5 s, %	19.0 19.69 *-3.5 %*	31.0 31.97 *-3.0 %*	14.3 14.60 *-2 %*	103.3 103.62 *-0.3 %*	103.8 103.94 *-0.1 %*	102.9 103.14 *-0.2 %*
Average Doppler Temperature at 5 s, °C	324.1 324.89 *-0.8 °C*	349.2 349.96 *-0.8 °C*	315.8 315.91 *-0.1 °C*	554.8 555.16 *-0.4 °C*	552.8 552.39 *+0.4 °C*	553.7 553.90 *-0.2 °C*
Max Fuel Centerline Temperature at 5 s, °C	672 679.30 *-7 °C*	556 559.66 *- 4 °C*	675 674.20 *+0.8 °C*	1688 1679.6 *+8 °C*	1556 1576.10 *-20 °C*	1724 1723.80 *+0.2 °C*

Coolant Outlet Temperature at 5 s, °C	293.1 293.22 *-0.1 ℃*	297.6 297.72 *-0.1 ℃*	291.54 291.53 *0.01 ℃*	325.7 324.90 *+0.8 ℃*	325.9 324.98 *+0.9 ℃*	325.6 324.77 *+0.8 ℃*

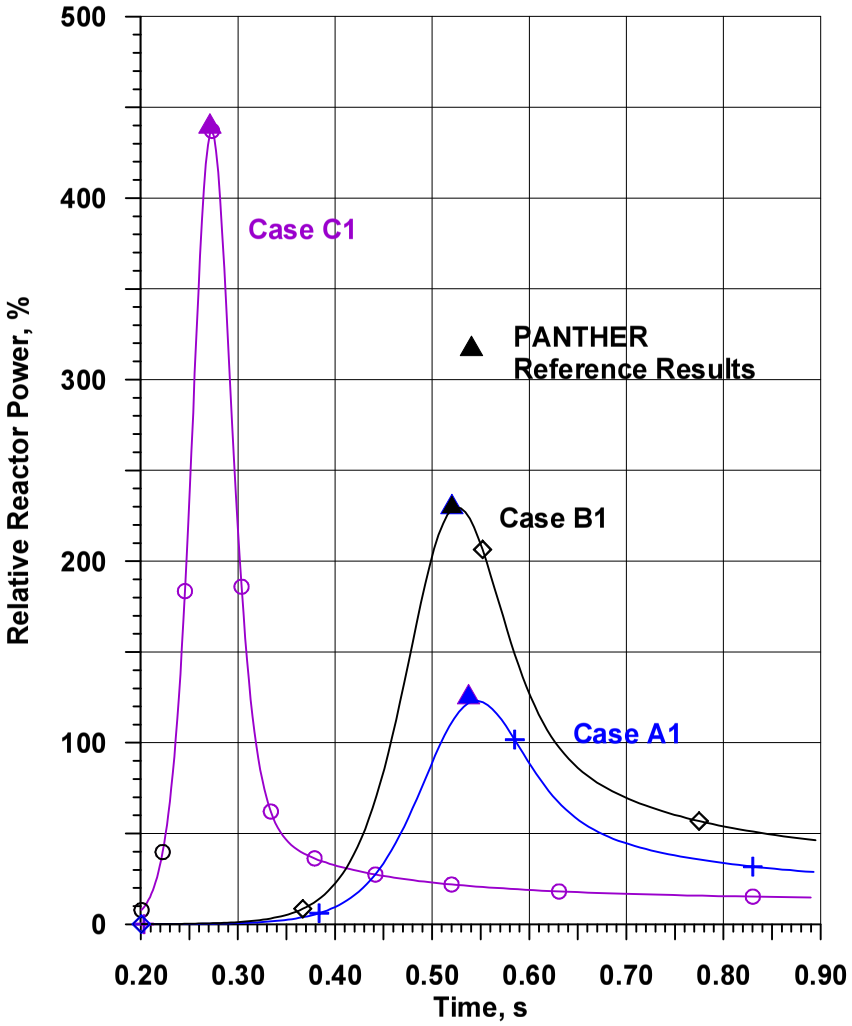

Fig. 5 Power versus time for the HZP cases A1, B1 and C1.

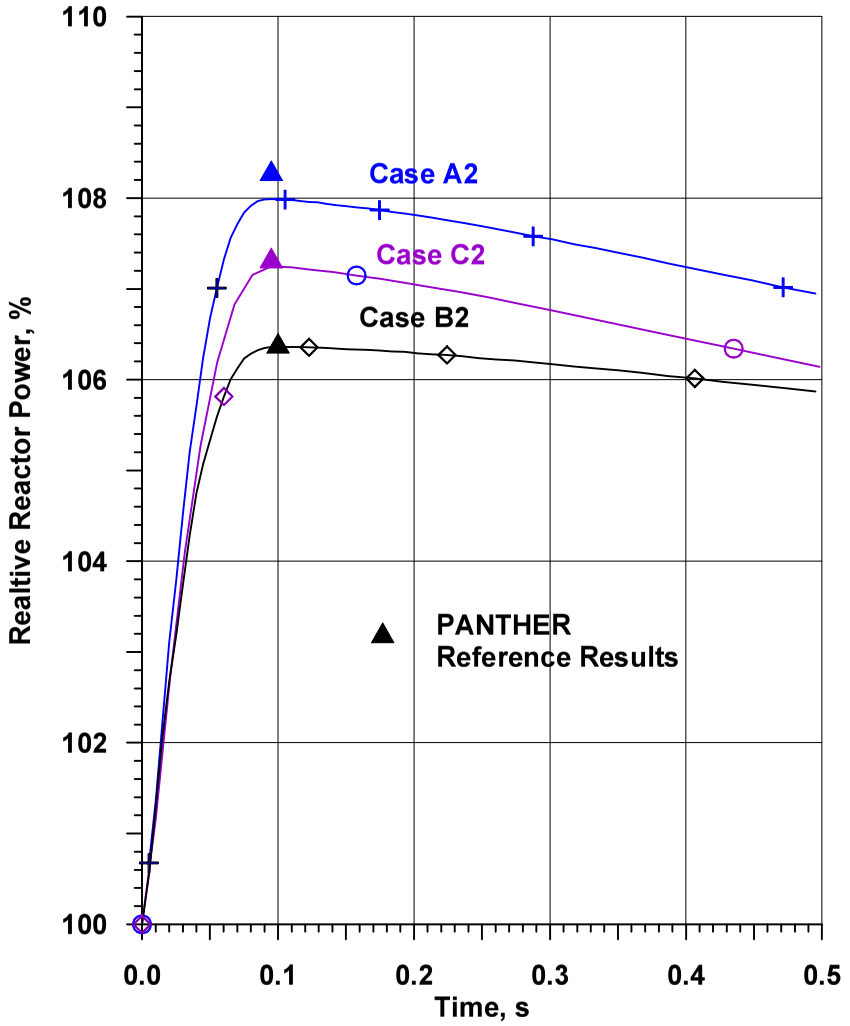

Fig. 6 Power versus time for the FP cases A2, B2, and C2.

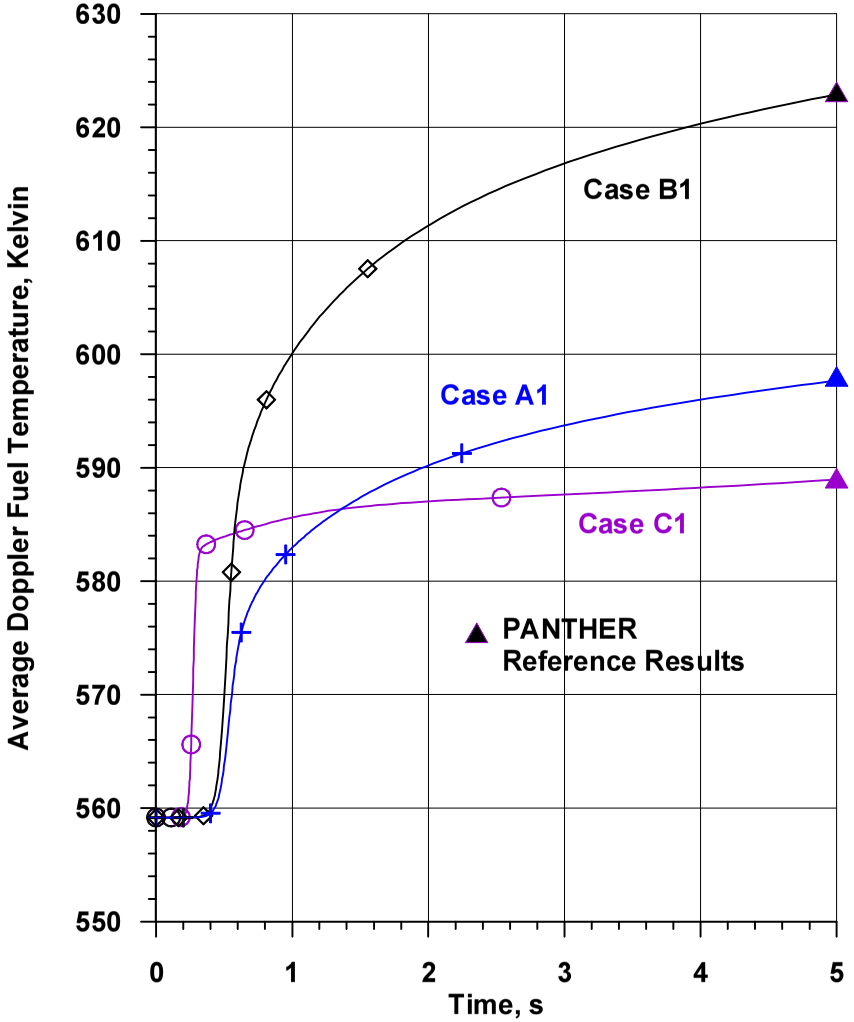

Fig. 7 Reactor-averaged Doppler fuel temperature versus time for the HZP cases A1, B1, and C1.

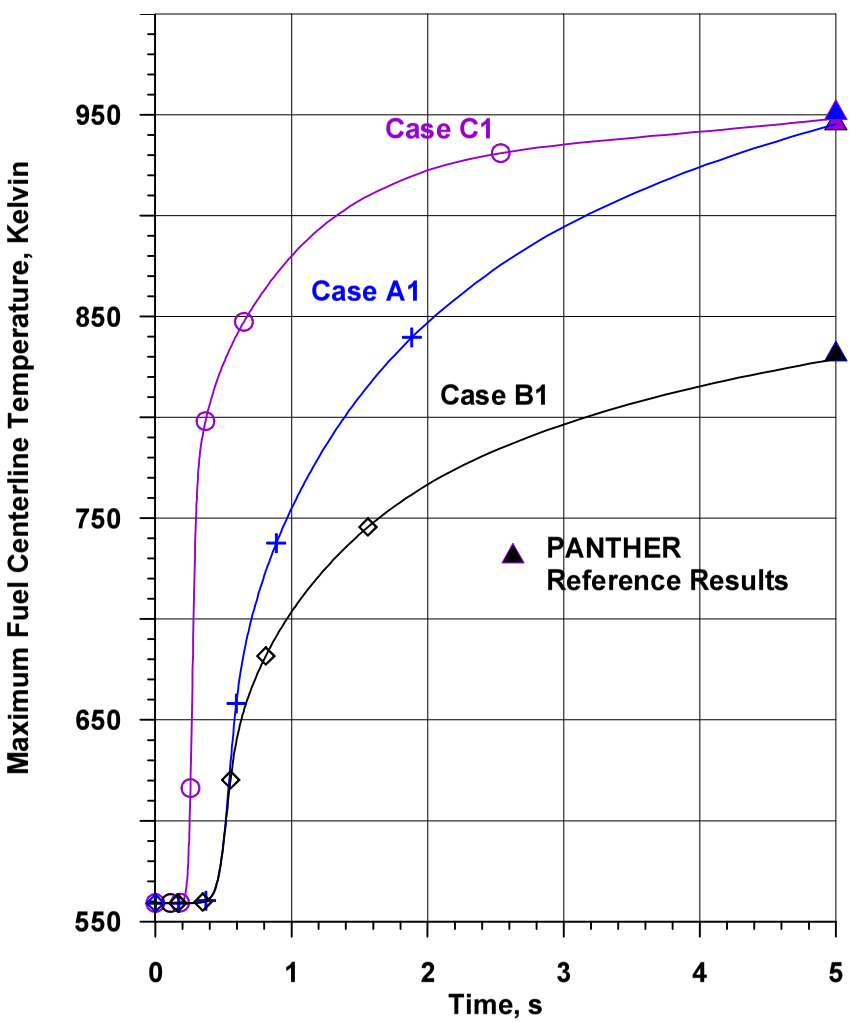

Fig. 8 Maximum fuel centerline temperature versus time for the HZP cases A1, B1, and C1.

The J-TRAC/SKETCH-N calculations were performed on a SUN Ultra 1 workstation with 143 MHz UltraSPARC processor. SunSoft FORTRAN 77 version 4.0 compiler was used. Computing time is 52 minutes for the case C1 (442x18 neutronics nodes, 88x14 thermal-hydraulics VESSEL nodes and 648 time steps). The SKETCH-N code takes about 65 % of the total computing time. An improvement of the SKETCH-N code efficiency is an area of the current efforts.

6. CONCLUSIONS

A three-dimensional neutron kinetics model has been implemented into the transient reactor analysis code J-TRAC to improve the code capabilities to simulate multidimensional space-time effects in a PWR core. The coupling is performed using the message-passing library PVM with minimum modifications of the both codes. The consistent mapping procedure, which provides the data transfer between the spatial meshes of the J-TRAC code and the neutronics mesh of the SKETCH-N code is developed. The verification of the coupled code system is performed against the NEACRP PWR rod ejection benchmark. A comparison of the results with the PANTHER reference solution demonstrates good accuracy in the all important transient parameters. The results show that the J-TRAC/SKETCH-N code system can be used for practical PWR REA calculations. The developed code system can be also useful for the other PWR transients where space-time effects in the reactor core are important: rod withdrawal accidents, main steam line breaks, boron dilution event etc.

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