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# Comparative analysis of neutronics/thermal-hydraulics multi-scale coupling for LWR analysis

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**Abstract**

The aim of the research described in this paper is to perform consistent comparative analyses of two different approaches for coupling of two-scale, two-physics phenomena in reactor core calculations. The physical phenomena of interest are the neutronics and the thermal-hydraulics core behaviors and their interactions, while the spatial scales are the "global" (assembly/channel-wise) and the "local" (pin/sub-channel-wise). The objective is three-fold: qualification of coupled code systems by consistent step-by-step cross-comparison (in order to understand the prediction deviations in both neutronics and thermal-hydraulics parameters); assessment of fine scale (local/subchannel-wise) thermal-hydraulic effects; and evaluation of the impact of on-line modeling of interactions of the two spatial scales. The reported work is within the cooperation between the Universidad Politécnica de Madrid (UPM), Spain and the Pennsylvania State University (PSU), USA. The paper first presents the two multi-scale coupled code systems followed by cross-comparisons for steady state calculations. Selected results are discussed to highlight some of the issues involved in comparative analysis of coupled multi-scale simulations. The transient comparisons are subject of future work and publications.

## 1. Introduction

Design margins could be improved by integrated high-fidelity reactor core simulations, which involve modeling of neutronics, fluid and heat transfer (thermal-hydraulics), thermo-mechanics, and fuel behavior – all with feedback effects. A code system capable of such simulations must take into account the coupling of different physical phenomena (multi-physics) at different spatial and time scales (multi-scale) during reactor operation and safety related transients.

The aim of the research described in this paper is to perform consistent comparative analyses of two different approaches for coupling of two-scale, two-physics phenomena in reactor core calculations. The physical phenomena of interest are the neutronics and the thermal-hydraulics core behaviors and their interactions, while the spatial scales are the "global" (assembly/channel-wise) and the "local" (pin/sub-channel-wise). The objective of such comparative

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analysis is three-fold: qualification of coupled code systems by consistent step-by-step cross-comparison (in order to understand the prediction deviations in both neutronics and thermal-hydraulics parameters); assessment of fine scale (local/sub-channel-wise) thermal-hydraulic effects; and evaluation of the impact of on-line modeling of interactions of the two spatial scales. The reported work is within the cooperation between the Universidad Politécnica de Madrid (UPM), Spain and the Pennsylvania State University (PSU), USA.

Both organizations have accumulated significant experience and expertise in developing core neutronics/thermal-hydraulics coupling schemes for reactor design and safety analysis. Their current work is focused on implementation of optimized on-line spatial two-scale two-physics coupling methodologies. The motivation for such efforts is the fact that the "global" core models do not have sufficient resolution to predict "local" coupled effects, which are important for the fuel design safety margins. In achieving this objective the two organizations have selected two different approaches.

## 2. Coupled code systems

### *2.1. UPM system*

The UPM advanced multi-scale neutron-kinetics (NK) and thermal-hydraulics (TH) methodology, being implemented in the code system COBAYA3 (Aragonés J.M. et al., 2005), includes domain decomposition by alternate core dissections for the local three-dimensional (3D) fine-mesh scale problems (pin cells/sub-channels) using a 3D multi-group transport corrected method. For the assembly-wise scale an analytical nodal diffusion solver (ANDES) is being used, which has also been developed during the last years, within our research group, under the European project NURESIM (Zerkak O. et al., 2007).

Nowadays, the thermal-hydraulic codes used to perform coupled calculations at both scales are COBRA-IIIc/MIT-2 and COBRA-TF (joint PSU-UPM version). The COBRAIIIc/MIT-2 sub-channel code has been extensively utilized as a TH solver within the previous UPM codes for PWR core simulation (Aragonés J.M. et al., 2004). Later, due to its advanced physical models, COBRA-TF sub-channel code was introduced as an alternative option. While the fluid solution of COBRAIIIc/MIT-2 is based on the homogeneous mixture model, COBRA-TF features two-fluid (vapor and liquid) three-fields (continuous vapor, continuous liquid, and entrained liquid) representation of the two-phase flow. The code also considers reversed flow situations. Regarding the heat transfer solution, COBRA-TF allows radial, axial, and azimuthal heat conduction in comparison to only radial conduction modeled in COBRAIIIc/MIT-2. Also, a dynamic gap heat transfer model is available in COBRA-TF. In other words, COBRA-TF offers more modern physics for modeling of time-dependent phenomena in highly heterogeneous nuclear reactor cores. However, because of its faster numerics, COBRAIIIc/MIT-2 is the preferable TH solver for steady-state and transient single-phase flow calculations.

The COBAYA3 source code structure is based on the idea of generating a unique executable where each solver (either neutronic or thermal-hydraulic) is encapsulated with some inputs and outputs. Therefore, the NK-TH coupling is performed via internal common memory (Figure 1); this memory can be seen as coupling interfaces in which variables are shared between the codes.

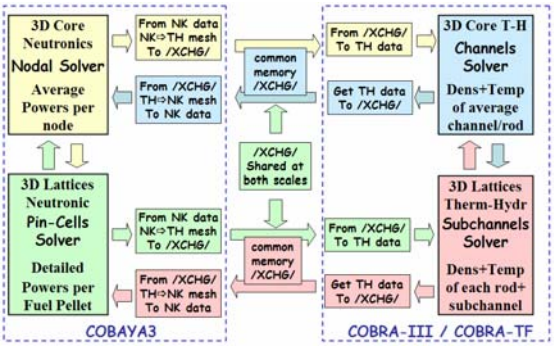



Fig. 1. Multi-scale and multi-physics coupling in the UPM code system.

The necessary mesh transformations in a coupled calculation are included in the neutronic part of COBAYA3, which requires some extra input data to define the TH meshing. Apart from that, an input data pre-processor was developed in order to generate the full input deck for both TH codes. Those inputs decks are automatically generated for each coupled calculation what helps to assure that the geometry has been setup properly.

The top part of the Figure 1 represents the calculation path in a coupled NK-TH calculation at coarse mesh scale. ANDES (Lozano J.A. et al., 2008) is a multi-group analytical nodal diffusion solver based on the Analytical Coarse Mesh Finite Difference (ACMFD) method. This neutronics solver supports Cartesian and hexagonal configurations and has been validated running several exercises of the well-known OECD/NEA benchmarks, such as the control rod ejection or bank withdrawal. At the global scale, the coupled steady state and transient calculations are performed using one of the mentioned TH codes and applying the hypothesis of average channels selecting 1 or 4 channels per assembly.

The bottom part of the Figure 1 represents the calculation path for coupled calculation at local fine-mesh scale. COBAYA3 has implemented a coupling scheme that supports the domain decomposition by alternate core dissections methodology (Herrero J.J. et al., 2007). The aim of this methodology is to accelerate the whole convergence of the fine-mesh calculations by a coarser mesh solution performed by ANDES, which is computed after each solution of all the core sub-domains belonging to one kind of partition of the problem at a time, generating a sequence of fine(m)—coarse—fine(n) mesh solutions through the process, where m and n refer to different kinds of partitions of the core. First, a solution in a coarser scale transports long wavelength effects; and this will be reflected in the next fine mesh iteration by modifying the boundary conditions with the nodal solution values. The detailed boundary conditions are updated with the difference arising from the new nodal current to flux ratios of the converged nodal solution, while maintaining the detailed profile of the previous fine mesh iteration. The nodal solution will update the normalization of fission sources improving the full core power normalization.

### *2.2. PSU system*

The PSU multi-scale coupled scheme is based on an embedded pin-by-pin local fuel assembly calculation within the framework of a core assembly-wise simulation. Both scales are analyzed with the same neutronics (NEM) and thermal-hydraulics (COBRA-TF) modules within the framework of the coupled multi-physics code system CTF/NEM. The NEM version applied to local pin-by-pin calculations is named NEML.

The PSU coupled multi-physics code system CTF/NEM is based on the joint PSU-UPM version of COBRA-TF code and the PSU version of NEM code. During the last few years, the theoretical models and numerics of the advanced two-fluid, three-field sub-channel code COBRA-TF have been substantially improved (Cuervo D. et al., 2005 and Avramova M. et al., 2006). The code has been subjected to an extensive verification and validation program and has been applied to variety of Light Water Reactor (LWR) steady state and transient simulations. The Nodal Expansion Method (NEM) diffusion code has been developed, maintained, and continuously enhanced at PSU. NEM (Beam T. et al., 1999) is a few-group (with up to 10 energy groups) 3D steady-state and transient nodal core model with three geometry modeling options: Cartesian, Hexagonal-Z, and Cylindrical (R-θ-Z). The code is based on transverse integration procedure and it was updated to utilize semi-analytical transverse-integrated flux representation and improved transverse leakage approximation. The time dependence of the neutron flux is approximated by a first order fully implicit finite-difference scheme (upgraded later with exponential transformation technique), whereas the time dependence of the neutron precursor distributions is modeled by a linear time-dependent approximation. Recently, $SP_3$ transport option was implemented within the framework of NEM.

NEM is coupled with COBRA-TF in serial integration manner (Tippayakul C. et al., 2007) (in fact NEM is incorporated as a subroutine in the COBRA-TF calculation flow). The CTF/NEM code system is designed to provide a platform for implementation of direct and embedded multi-scale algorithms in space and time domains of coupled simulations. The multi-scale scheme proposed in this work is based on embedded local coupled fuel assembly calculation within the framework of the coupled core calculation. This is a non-linear iteration process, which involves averaging and reconstruction procedures, boundary conditions evaluation and exchange, and pre-passing of correction parameters between two spatial scales (global solution and local calculation) for both physical phenomena – neutronics (Ivanov B. et al., 2007) and thermal-hydraulics. The embedded multi-scale coupling scheme of NEM/CTF is shown in Figure 2.

### 2.3. *Efficiency of coupled two-scale calculations*

Improving the efficiency of coupled multi-scale calculations is very important for practical applications. The UPM and PSU code systems utilize in different manner non-linear iterations between the two scales combined with using acceleration strategies and parallel computing. PSU in collaboration with UPM has improved the stand-alone COBRA-TF computational efficiency by implementing an optimized matrix solver, based on pre-conditioned Krylov non-stationary iterative methods. This implementation has been extended to the coupled NK-TH calculations.

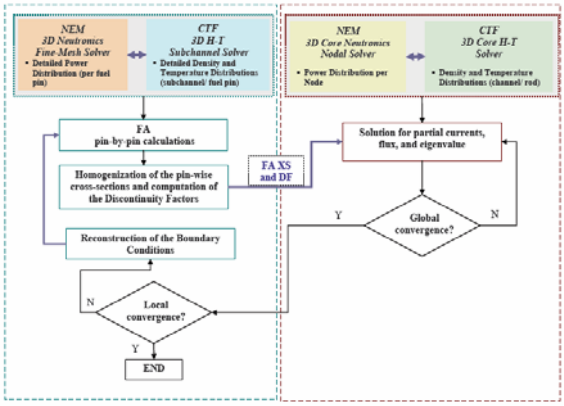



Fig. 2. Multi-scale and multi-physics coupling in the PSU code system

COBRA-TF, as originally developed, provides two options for faster achievement of a steady state solution. First, to minimize the expensive "null-transient" time, a calculation of steady state rod temperatures can be requested. Also, via an input specification, the time step size for the solution of the conduction equation can be defined larger than the fluid solution time step size. The latter can significantly reduce the CPU time needed to reach steady state, but the calculated radial distributions of the fuel temperature may differ. Therefore, the next step should be a development of a steady state solution option in the COBRA-TF numerics.

## 3. Comparative analysis

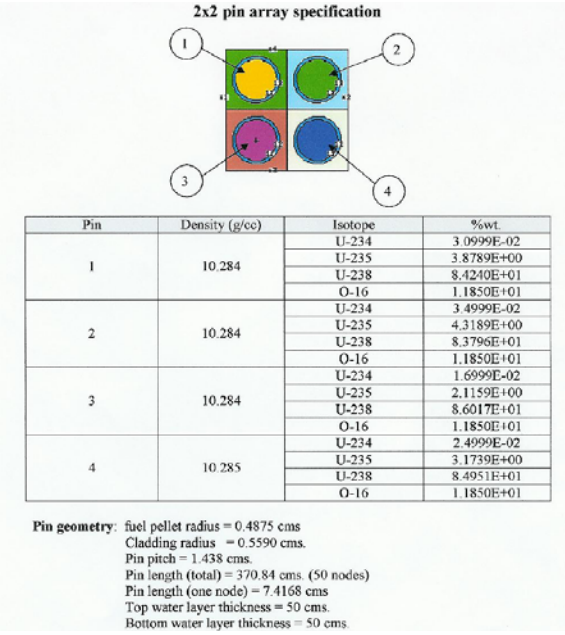
The comparative analysis between the two code systems reported in this paper is for steady state calculations. The transient comparisons are subject of future work and publications. Several test problems were designed or utilized from the published literature to address stand-alone and coupled models' verification on both local and global spatial scale. On local level these problems include 3D 2x2 pin array, a 3D assembly model, and a 3D 2x2 assembly color-set. On global level the test problems include a 3D 2x2 assembly color-set, a whole core calculation (based on the *OECD/NEA PWR Rod Ejection Analysis (REA) benchmark*, Finnemann H., 1992), and a second whole core calculation (based on *OECD/NRC PWR Main Steam Line Benchmark (MSLB) benchmark*, Ivanov K., 1999). The cross-section libraries were either utilized form the published benchmarks or generated at PSU with CASMO-3 (Forssen B. et al., 1992) or HELIOS (StudsvikScandpower, 2001). First, the so-called "direct" (single-scale) calculations are compared between the two code systems for the two spatial scales on the test problems described above starting from stand-alone neutronics and stand-alone thermal-hydraulics calculations and completing the first step with coupled calculations. Such approach helps to identify and understand the deviations in a consistent manner. In the second step of the comparative analysis two-scale (utilizing non-linear iterations between the two scales) stand-alone neutronics and subsequently coupled calculations are performed for the 3D 2x2 assembly color-set. Selected results are presented in this paper to highlight some of the issues involved in comparative analysis of coupled multi-scale simulations.

Stand-alone neutronics comparisons on local level for a 3D 2x2 pin array with 60 axial nodes (extracted from a BWR assembly) demonstrated very good agreement between neutronic solvers of the UPM and PSU systems. The two-group cross-sections were generated with CASMO-3 using geometry and material data shown in Figure 3. Each pin axially was represented by one material plus bottom and top axial reflector. Reflective boundary conditions are used in radial plane and zero flux boundary conditions are used in axial direction. The $k_{eff}$ and radial power distribution comparisons are given in Tables 1 and 2 while axial power distributions are compared in Figure 4.

The stand-alone comparisons on global/assembly level are shown for a PWR mini-core problem (Case 1a) developed in (Ivanov B. et. al., 2006). This is a 3x3 2D problem in Cartesian geometry consisting of one rodded central assembly surrounded by eight unrodded assemblies. The assembly homogenized cross-sections are also

generated by CASMO-3 and are divided by assembly discontinuity factors. The $k_{eff}$ comparisons are shown in Table 3 while the 2D power distribution comparison is shown in Table 4.

It is known that in coupled calculations, the prediction of the thermal-hydraulic feedback parameters (which affect subsequently the prediction of neutronic parameters) depends on the fuel rod model (for Doppler temperature) and steam-water property tables (for moderator density) utilized in the thermal-hydraulic code. Such dependence was observed also in our comparative analysis when using two different thermal-hydraulics codes - COBRAIIIc/MIT-2 and COBRA-TF – as feedback models. The effect of fuel rod modeling was analyzed on both global and local spatial scale.




| Pin | Density (g/cc) | Isotope | %wt. |
|---|---|---|---|
| 1 | 10.284 | U-234 | 3.0999E-02 |
| | | U-235 | 3.8789E+00 |
| | | U-238 | 8.4240E+01 |
| | | O-16 | 1.1850E+01 |
| 2 | 10.284 | U-234 | 3.4999E-02 |
| | | U-235 | 4.3189E+00 |
| | | U-238 | 8.3796E+01 |
| | | O-16 | 1.1850E+01 |
| 3 | 10.284 | U-234 | 1.6999E-02 |
| | | U-235 | 2.1159E+00 |
| | | U-238 | 8.6017E+01 |
| | | O-16 | 1.1850E+01 |
| 4 | 10.285 | U-234 | 2.4999E-02 |
| | | U-235 | 3.1739E+00 |
| | | U-238 | 8.4951E+01 |
| | | O-16 | 1.1850E+01 |

**Pin geometry**: fuel pellet radius = 0.4875 cms
Cladding radius = 0.5590 cms.
Pin pitch = 1.438 cms.
Pin length (total) = 370.84 cms. (50 nodes)
Pin length (one node) = 7.4168 cms
Top water layer thickness = 50 cms.
Bottom water layer thickness = 50 cms.

Fig. 3. 2x2 pin array test problem specifications

Table 1
$k_{eff}$ comparisons for 3D 2x2 pin array test problem

| Code | NEM | COBAYA3 ANDES | COBAYA3 LATTICE |
|---|---|---|---|
| $k_{eff}$ | 0.89402 | 0.89404 | 0.89401 |

Table 2
Radial power distribution comparison for 3D 2x2 pin array test problem

NEM

| | 1 | 2 |
|---|---|---|
| 1 | 1.1055 | 1.1399 |
| 2 | 0.7756 | 0.9790 |

COBAYA3 ANDES

| | 1 | 2 |
|---|---|---|
| 1 | 1.1055 | 1.1399 |
| 2 | 0.7756 | 0.9790 |

COBAYA3 LATTICE

| | 1 | | 2 | |
|---|---|---|---|---|
| 1 | 1.1018 | 1.1026 | 1.1379 | 1.1388 |
| | 1.1081 | 1.1079 | 1.1411 | 1.1410 |
| 2 | 0.7751 | 0.7738 | 0.9790 | 0.9771 |
| | 0.7785 | 0.7767 | 0.9814 | 0.9787 |

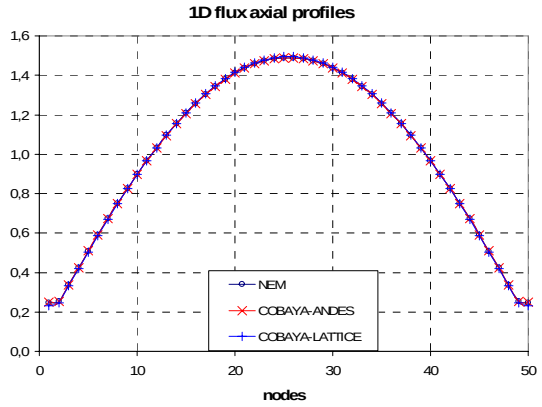



Fig. 4. Axial power distribution comparison

Table 3
$k_{eff}$ comparisons for 2D 3x3 assembly configuration

| Test 1a | 1 node per FA | 4 nodes per FA |
|---|---|---|
| CRONOS $k_{eff}$ | 1.06892 | 1.06894 |
| NEM $k_{eff}$ | 1.06917 | 1.06896 |
| ANDES $k_{eff}$ | 1.06897 | 1.06895 |

Table 4
Radial power distribution comparison for 2D 3x3 assembly configuration

| 1 node per FA | | | 4 nodes per FA | | | |
|---|---|---|---|---|---|---|
| 1.0640 | 1.0110 | 1.0640 | 1.0640 | 1.0110 | 1.0640 | |
| 1.0607 | 1.0165 | 1.0607 | 1.0640 | 1.0114 | 1.0640 | |
| 1.0637 | 1.0117 | 1.0637 | 1.0641 | 1.0112 | 1.0641 | |
| 1.0110 | 0.6991 | 1.0110 | 1.0110 | 0.6981 | 1.0110 | CRONOS |
| 1.0165 | 0.6912 | 1.0165 | 1.0114 | 0.6985 | 1.0114 | NEM |
| 1.0117 | 0.6981 | 1.0117 | 1.0112 | 0.6988 | 1.0112 | ANDES |
| 1.0640 | 1.0110 | 1.0640 | 1.0640 | 1.0110 | 1.0640 | |
| 1.0607 | 1.0165 | 1.0607 | 1.0640 | 1.0114 | 1.0640 | |
| 1.0637 | 1.0117 | 1.0637 | 1.0641 | 1.0112 | 1.0641 | |

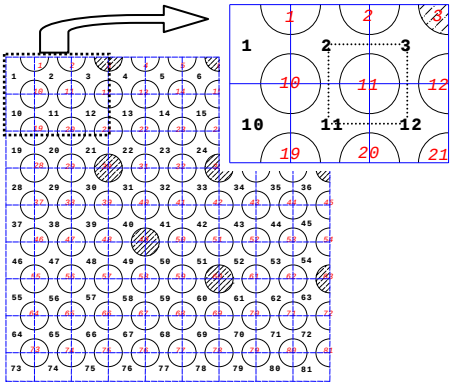


Fig 5. Coupling discretization scheme at pin cell level

On the local scale, four subchannels surrounding each pin cell (see Figure 5 for more details) were utilized for the two cases presented here. The cases correspond to 3D models of one assembly and one assembly color-set with different fuel configurations. COBRA-TF results were obtained using the constant gap conductance model with a given gap conductivity as well as the dynamic gap conductance model also available in the code. COBRAIIIc/MIT-2 results are obtained only with the specified constant gap conductance model since the code does not have a dynamic gap conductance model. The 3D assembly model is extracted from the PWR MOX benchmark (Kozlowski, T. et al., 2003) and the results shown in Table 5 are calculated with the coupled COBAYA-3 lattice solver with COBRAIIIc and COBRA-TF. The assembly test model consists of 289 pin cells in radial plane and 136 axial layers and 8-group pin-wise cross-section tables were used. The constant gap conductance model was utilized with a gap conductivity of 10000 W/m$^2$K. The case has been analysed at nominal operating conditions.

Further, the 3D single assembly model was extended to 3D 2x2 assembly color-set (324 pin cells in the radial plane) problem using the same PWR MOX benchmark cross-section libraries but with different materials compositions. A two colors color-set was computed with reflective boundary conditions in the radial direction (infinite core) and void in the axial direction. The same mesh-refinement as in the previous case was used. The obtained results with the lattice solver are shown in Table 6.

Table 5
3D assembly model comparisons

| ASSEMBLY | $k_{eff}$ | $F_z$ | $F_{xy}$ | $Tf_{dop}$ [1] | $Tf_{surf}$ [2] | $Tf_{max}$ [3] |
|---|---|---|---|---|---|---|
| COBRA-TF Constant gap conductance model | 0.93356 | 1.447 | 1.0578 | 548.8 | 437.5 | 1170.9 |
| COBRA-TF Dynamic gap conductance model | 0.93291 | 1.463 | 1.0579 | 575.5 | 461.7 | 1190.8 |
| COBRA-IIIc | 0.93363 | 1.446 | 1.0577 | 553.7 | 427.0 | 1199.8 |

On the global scale the same 3D 2x2 color-set was analyzed but now with ANDES using 4 nodes per assembly and COBRAIIIc and COBRA-TF using also 4 thermal-hydraulic channels per assembly (a quarter of assembly per channel). In the axial directions 34 nodes were utilized (each node at global level is equivalent to 324 cells in the detailed calculation for both N and TH meshes). The comparison of results is shown in Table 7.

Table 6
3D color-set model comparisons at local level

| COLORSET | $k_{eff}$ | $F_z$ | $F_{xy}$ | $Tf_{dop}$ | $Tf_{surf}$ | $Tf_{max}$ | $U_{ave}$ [4] |
|---|---|---|---|---|---|---|---|
| COBRA-TF Constant gap conductance model | 1.04645 | 1.492 | 1.2957 | 550.9 | 438.1 | 1487.7 | 0.7013 |
| COBRA-TF Dynamic gap conductance model | 1.04579 | 1.512 | 1.2953 | 575.5 | 460.0 | 1445.7 | 0.7012 |
| COBRA-IIIc | 1.04629 | 1.490 | 1.2948 | 566.4 | 392.2 | 1670.5 | 0.7044 |

Table 7
3D color-set model comparisons at global level

| COLORSET with ANDES | $k_{eff}$ | $F_z$ | $F_{xy}$ | $Tf_{dop}$ | $Tf_{surf}$ | $Tf_{max}$ | $U_{ave}$ |
|---|---|---|---|---|---|---|---|
| COBRA-TF Constant gap conductance model | 1.04462 | 1.477 | 1.1504 | 544.0 | 432.1 | 1262.2 | 0.7025 |
| COBRA-TF Dynamic gap conductance model | 1.04200 | 1.480 | 1.1504 | 628.7 | 508.9 | 1382.3 | 0.7026 |
| COBRA-IIIc | 1.04448 | 1.475 | 1.1511 | 559.2 | 422.2 | 1406.0 | 0.7043 |

As seen from Tables 5, 6, and 7 there are two major disagreements in the predictions of COBRA-IIIc and COBRA-TF.

First, COBRAIIIc always calculates steeper

[1] $Tf_{dop}$: Average fuel Doppler temperature in the problem (ºC)
[2] $Tf_{surf}$: Average fuel surface temperature in the problem (ºC)
[3] $Tf_{max}$: Maximum fuel temperature in the problem (ºC)
[4] $U_{ave}$: Average density in the problem (g/cm$^3$)

radial temperature profile inside the fuel pellet. This might be explained with the fuel rod models utilized in the codes. Both assume boundary conditions of no heat flow across the centerline, but use different nodalizations to solve the heat conduction equation. In COBRA-IIIc, the equation is directly solved at the fuel center by applying the L'Hospital's rule. In COBRA-TF, because the conduction node for the center region is located off the centerline, the centerline temperature is defined by Hermite interpolation.

Second, the dynamic gap conductance model in COBRA-TF leads to prediction of higher fuel pellet surface temperature. As a sequence, higher Doppler temperature is calculated which results in a lower multiplication factor in the coupled calculations. Also, while using the dynamic gap conductance model, the greatest discrepancies are found at the global level. It seems that the heat transfer models using a dynamic gap conductance in COBRA-TF are more accurate when one rod is modeled as single pin rather than when a rod represents an assembly (at global scale). Therefore, the dynamic gap conductance model was not considered in the performed PWR REA and PWR MSLB calculations, where each FA is modeled by a single sub-channel/rod.

As expected, the highest peak power is given by the lattice calculation (see $Tf_{max}$) because of the detailed geometry representation. Comparing COBRA-TF between local and global level, it can be seen that the results obtained using dynamic gap conductance model are more different between both scales. However, using the constant gap conductance model those are closer between different scales and also closer with COBRA-III. The $k_{eff}$ discrepancies between the global and the local level cases are not larger than 200 pcm. We have run the same color-set cases without coupling and the discrepancies in $k_{eff}$ were about 100 pcm. So about the half of the discrepancy comes from the fact that the assembly discontinuity factors (ADF's), that are been used by ANDES, where calculated for isolated assemblies (in infinite geometry) rather than for color-set configuration and the other half is due to the TH feedback effect. The best performance of COBRA-TF is obtained using the constant gap conductance model when comparing against COBRA-IIIc.

Next results obtained with a full core model at global level are presented in Table 8 and discussed. The core model is using one channel per assembly, and it corresponds to the first exercise of the OECD/NEA REA benchmark for PWR (which specifies a constant gap conductance model with a given gap conductivity value). Please note that the power was introduced in COBRA-TF as a 3D power distribution extracted from the converged COBAYA3/COBRA-III solution. The used criteria to determine if the steady state has been achieved by the COBRA-TF calculation was 0.2% of error in both mass and heat conservation equations. In this sense, the COBAYA3/COBRA-TF results in Table 8 provide the COBRA-TF response to the given 3D power distribution. The obtained results confirm that COBRA-TF predicts lower Doppler temperature than COBRA-III. The coupled NEM/COBRA-TF (CTF/NEM) calculations predict lower Doppler and moderator temperatures as compared to COBRA-III. The latter is due to different tables of physical properties of water used in both codes. Since the Doppler temperature and the moderator temperature have negative feedback effects on the multiplication factor, the NEM/COBRA-TF coupled calculation gives a higher multiplication factor than COBAYA3/COBRA-III.

Table 8
PWR REA HFP comparison

| Case B2 HFP | $k_{eff}$ | $Tf_{dop}$ | $Tf_{max}$ | $Tc_{max}$ [5] | $Tw_{out}$ [6] | $Tw_{max}$ [7] |
|---|---|---|---|---|---|---|
| REFER. | 1.00000 | 543.7 | 1576.6 | - | - | - |
| COBAYA3 COBRA-III | 1.00056 | 543.6 | 1574.5 | 346.7 | 324.1 | 329.2 |
| COBAYA3 COBRA-TF | 0.99818 | 498.2 | 1493.2 | 346.8 | 322.7 | 328.1 |
| NEM COBRA-TF | 1.00103 | 495.9 | 1475.3 | 347.4 | 323.2 | 328.8 |

The last test problem discussed in this paper is based on the OECD/NRC PWR MSLB calculations. The results are compared at the initial HFP steady state conditions and shown in Table 9. The comparative analysis of this table confirms the tendencies observed in Table 8.

Regarding comparisons to reference values, it has to be highlighted that the references are either calculated by a given spatially converged "trusted" code (REA benchmark) or taken as an average of

[5] $Tc_{max}$: Maximum cladding temperature in the problem (ºC)
[6] $Tw_{out}$: Average water temperature at the outlet (ºC)
[7] $Tw_{max}$: Maximum water temperature in the problem (ºC)

the participants results. Therefore, they are highly models dependent.

Table 9
PWR MSLB HFP comparison

| MSLB HFP | $k_{eff}$ | $Tf_{dop}$ | $Tf_{dopmax}$ [8] | $F_{xy}$ | $F_z$ |
|---|---|---|---|---|---|
| REFER. | 1.00490 | 549.8 | 674.8 | 1.3354 | 1.0858 |
| COBAYA3 COBRA-III | 1.00444 | 540.7 | 664.3 | 1.3088 | 1.0810 |
| COBAYA3 COBRA-TF | 1.00508 | 479.7 | 570.5 | 1.3085 | 1.112 |
| NEM COBRA-TF | 1.00513 | 467.3 | 565.3 | 1.3002 | 1.104 |

## 4. Conclusions

The reported study demonstrates that there are many open issues about the accuracy/adequacy of the nowadays used subchannel codes for coupled neutronics/thermal-hydraulic calculations. An example is the dynamic versus constant gap conductance modeling, which has proven to have significant effect on the Doppler temperature and consequently on the multiplication factor. It has to be noted that for the most of NEA/OECD benchmarks the gap conductivity for all the gaps is set to one value in all the rods (assemblies). However, in a real core, not all the assemblies are made of fresh fuel, and there are some once or twice burned assemblies. Those assemblies have lower gap conductivity and could be affecting the calculation done with the constant gap conductance model. In realistic calculation the dynamic gap conductance model is calibrated using a fuel performance code. The future plans include coupling COBRA-TF to FRAPCON (Berna G.A. et al., 1997) for steady state calculations and FRAPTRAN (Cunningham M.E. et al., 2001) for transient applications. Additionally, it will be very beneficial to validate the nuclear fuel rod models of the subchannel codes against real experiments.

UPM and PSU have performed multi-scale standalone neutronics calculations with COBAYA3/ANDES (Herrero J.J. et al., 2007) and NEML/NEM (Ivanov B. et al., 2008). The 3D 2x2 assembly color-set (mini-core) problem is being used to compare the two systems first in stand-alone neutronics multi-scale calculations and then in coupled multi-scale calculations taking into account the results presented in this paper.

[8] $Tf_{dopmax}$: Maximum Doppler temperature in the problem (ºC)

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