Improvements and Applications of COBRA-TF for Stand-Alone and Coupled LWR Safety Analyses

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Abstract

The advanced thermal-hydraulic subchannel code COBRA-TF has been recently improved and applied for stand-alone and coupled LWR core calculations at the Pennsylvania State University in cooperation with AREVA NP GmbH, Germany and the Technical University of Madrid.

To enable COBRA-TF for academic and industrial applications including safety margins evaluations and LWR core design analyses, the code programming, numerics, and basic models were revised and substantially improved. The code has undergone through an extensive validation, verification, and qualification program.

KEYWORDS: COBRA-TF, subchannel analyses, computational efficiency, stand-alone and coupled calculations, safety margins evaluations

1. Introduction

In the past few decades, the need of improved nuclear reactor safety analyses has led to a rapid development of advanced methods for multidimensional thermal-hydraulic analyses. These methods have progressively become more complex in order to account for the many physical phenomena anticipated during steady-state and transient Light Water Reactor (LWR) conditions. In particular, the modeling of two-phase flow is especially complex. In two-phase flows, both thermal and mechanical non-equilibrium between the liquid and vapor phases exist. The non-equilibrium effects take the form of sub-cooled boiling, vapor superheating, and relative motion of the two phases. In order to have realistic calculations, all these physical phenomena must be accounted for in the theoretical models of a given computer code. The methods must be able to calculate the many flow patterns that occur in the postulated transients.

The advanced thermal-hydraulic subchannel code COBRA-TF [1-2] is widely used for best-estimate evaluations of the nuclear reactor safety margins. The original version of the code was developed at the Pacific Northwest Laboratory as a part of the COBRA/TRAC thermal-hydraulic code. Since then, various academic and industrial organizations adapted, developed, and modified the code. Recently COBRA-TF has been improved and applied for

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stand-alone and coupled reactor core calculations at the Pennsylvania State University (PSU) in cooperation with AREVA NP GmbH, Germany and the Technical University of Madrid (UPM).

2. COBRA-TF Features and Improvements

COBRA-TF (COolant Boiling in Rod Arrays – Two Fluid) features two-fluid, three-field representation of the two-phase flow and is applicable for both Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR) analyses. The three-fields are continuous vapor, continuous liquid, and entrained liquid drops in an annular flow. For each space dimension COBRA-TF solves three momentum conservation equations, four mass conservation equations, and two energy conservation equations. The code can handle both hot wall and normal flow regimes and can calculate reverse flow and cross-flow situations. The conservation equations for each of the three fields and for the heat transfer from and within the solid structure in contact with the fluid are solved using a semi-implicit, finite-difference numerical technique on an Eulerian mesh. The code features extremely flexible nodding for both thermal-hydraulic and heat-transfer solution. This flexibility allows modeling of a wide variety of geometries encountered in the vertical components of a nuclear power reactor vessel.

2.1 Improvement of the COBRA-TF Computational Efficiency

One of the major drawbacks of the early developed subchannel codes is their poor computational efficiency. In terms of CPU time, the solution of the system of linear equations that relate pressure in each cell of the computational mesh is the most important step in the solution process. There are two numerical methods originally implemented in COBRA-TF: direct inversion (Gaussian elimination) and Gauss-Seidel iterative technique. The first one is only recommended for cases with a small number of cells. The second one belongs to the group of stationary iterative methods.

In order to improve the code computational efficiency, two optimized matrix solvers, Super LU library [3] and Krylov non-stationary iterative methods [4] were successfully implemented in COBRA-TF for the solution of the linear system of pressure equations [5].

A suit of five test cases, which differ by their computational mesh size and structure and the simulated conditions (steady state or transient), was established to study the new solvers' performance.

The *Embedded mesh* case is a flow reduction transient hot subchannel analysis of a PWR core containing 157 17×17 fuel assemblies (FA). The interior channels of the computational mesh are real thermal-hydraulic channels within an assembly. From interior to exterior different size lumped channels were modeled until reaching a quarter of the assembly size. The model consists of 7920 computational cells.

The PWR *MSLB* case simulates a PWR Main Steam Line Break (MSLB) transient. This is a whole core model, where each fuel assembly is represented by one thermal-hydraulic subchannel. The model includes 157 subchannels each divided into 40 equidistant axial nodes, which results in a matrix dimension of 6280 × 6280. The simulation includes the first 50 seconds after the scram event.

The *TMI FA* case is a Three Mile Island (TMI) fuel assembly model on a cell-by-cell (pin-by-pin) level. The fuel assembly is divided into 268 subchannels and 24 axial nodes. The

computational mesh consists of 6144 cells. This is a "null" transient simulation for 5 seconds.

The *Flow reduction* case represents a PWR core (157 17×17 FA) in a 1/8th sector of core symmetry. The hottest fuel assembly, which is located in the core center, is modeled on a cell-by-cell level while the rest of the core is modeled as a subchannel per a fuel assembly. The model consists of 56 subchannels each divided axially in 50 nodes (a matrix dimension of 2800 × 2800). A 50% loss of coolant transient was simulated. The total simulation time was 15 seconds: 5 seconds "null" transient followed by 10 seconds of flow reduction.

The *Steady State* case is a 1/8th of core symmetry PWR (157 17×17 FA) core sector modeled on a FA-by-FA level. The computational mesh consists of 26 subchannels (one subchannel per a fuel assembly) each of them divided into 50 axial nodes, which results in a 1300 × 1300 matrix to be solved. A "null" transient of 5 seconds was simulated.

The performed comparative analyses demonstrated that for large cases, the implementation of the bi-conjugate gradient stabilized method (Bi-CGSTAB) combined with the incomplete LU factorization with dual truncation strategy pre-conditioner reduced the total computational time by a factor of 3 to 5. Both new solvers converge smoothly regardless of the nature of simulated cases and the mesh structures. They show better accuracy comparing to the Gauss-Seidel technique for all investigated test cases.

Tab.1 summarizes the acceleration in the inner iterations time and the total CPU time as compared to the direct inversion. It can be seen that when using SuperLU library for the pressure matrix factorization, the acceleration gained in the inner iteration results in acceleration in the total CPU time of the same order of magnitude. However, this is obviously not true when an iterative method is utilized instead of the direct elimination. Generally several inner iterations are required to fulfill the convergence criterion. In COBRA-TF an inner iteration is considered converged if the maximum normalized error is less than 10^{-4}. Further in the process, if the outer iteration convergence is not obtained, the time step will be repeated leading sequentially to an increase of the total computational time. In our Gauss-Seidel calculations that is the reason for the lost of approximately half of the speed-up gained in the pressure matrix solution. Such poor outer iteration convergence was never observed when the Bi-CGSTAB solver was used. In the latter, the great acceleration in the pressure matrix solution resulted in total CPU time reduction with a factor between 3 and 5 for large matrices. This effect is due to the fact that the performance of the rest of code modules is not influenced by the implementation of Krylov solver. However, here it should be emphasized that, for instance, a whole reactor core transient calculation usually takes hours to be completed. Thus, a speed up in an order of 3 to 5 times is already a very significant achievement.

Table 1: Acceleration [(a)] of the inner iterations time and the total CPU time in comparison to Direct Inversion

Test Case / Matrix Size	**Super LU**		**Gauss-Seidel**		**Bi-CGSTAB**	
	Inner Iteration	*Total Time*	*Inner Iteration*	*Total Time*	*Inner Iteration*	*Total Time*
Embedded mesh / 7920 × 7920	1.94	1.67	1.11	0.92	15.54	4.66
MSLB / 6280 × 6280	2.03	1.63	4.19	1.07	22.33	3.33
TMI FA / 6144 × 6144	2.97	2.23	2.14	2.69	9.29	4.91
Flow Reduction / 2800 × 2800	0.75	0.87	0.04	0.05	4.5	1.44
Steady State / 1300 × 1300	0.33	0.86	0.50	0.76	0.50	0.92

2.2 COBRA-TF Coding and Models Improvements

The original version of COBRA-TF was written for a UNIX operative system (CDC 7600). Later the source was adapted for a PC environment by removing machine dependent features and some old non-standard FORTRAN statements. However, the code was based on a static allocation memory and a special header file was used to set the dimensions of the arrays through PARAMETER operators. In order to enhance code performance, the code was recently translated to the FORTRAN90 language [6]. The FORTRAN90 dynamic allocation memory option is preferable to the static allocation memory because of the optimized memory usage. It was observed that the introduction of the FORTRAN90 features additionally speed-up the code by approximately a factor of 2.

During the COBRA-TF validation for LWR analyses several modifications were introduced [6]. Modifications were performed to improve the code capability of simulating a MSLB transient - possibility of time variations of the radial and axial power profiles was introduced. A model for a direct coolant heating was implemented as well. The user can specify by the input the heat fraction that will be generated into the coolant.

To improve and enhance the code capability of simulating both single and two-phase turbulent mixing and net transverse mass, energy, and momentum exchange between adjacent subchannels, the COBRA-TF turbulent mixing and void drift models were revised and improved [6]. The exchange of mass, energy, and momentum between adjacent subchannels is accounted for in the COBRA-TF balance equations for both single and two-phase conditions. The code internally calculates transverse fluctuating flow rate per unit length across the gap between the subchannels based on diversion, mixing and void drift effects. In the current model, the single-phase mixing coefficient can be either an input specified value or calculated using Rogers and Rosehart correlation [7]. For two-phase flow conditions, the turbulent mixing enhancement is modeled utilizing the work of Beus [8] and Wallis [9] and the Lahey's void drift model [10]. The new COBRA-TF turbulent mixing and void drift models were validated [6] against two rod bundle experiments, GE Nine-Rod Bundle Experiment [11] and Joint Research Center ISPRA PELCO-S Sixteen-Rod Bundle Experiment [12].

3. Stand-Alone COBRA-TF PWR Applications

An extensive COBRA-TF validation program for PWR stand-alone applications was defined and successfully completed [6, 13-14]. The related activities consist of two major parts: standard PWR applications and challenging PWR applications.

The simulated reactor core was representative of a typical PWR and consisted of 157 17×17 fuel assemblies, each of them containing 264 fuel rods and 25 guide tubes. One-eight symmetry core calculations were performed on two levels, core wide and fine subchannel. The first core model (FA-by-FA model) represents each fuel assembly as one subchannel, which contains a "pseudo" fuel rod with a radial power factor equal to the normalized assembly power factor. In the second core representation (cell-by-cell model) the hot fuel assembly, which is situated in the center of the core, is modeled in a detailed cell-by-cell approach. In axial direction for both core models each subchannel is divided into 40 equidistant nodes. The core thermal-hydraulic boundary conditions were provided by the TRAC-PF1 thermal-hydraulic system code, while the core radial power distribution was obtained by the NEM 3D neutron-kinetics code [15]. The axial heat flux distribution is

modeled as a chopped cosine with a peak value of 1.55. The inlet mass flow rate (according to the subchannel cross-sectional area) and enthalpy are applied as inlet boundary conditions. The system pressure is applied as outlet boundary condition. The model includes lower and upper tie plates, two structural spacers, and six mixing spacers.

Steady-state calculations at different core powers and transient calculations of flow reduction (pump coast-down), power rise (bank withdrawal at power), and pressure reduction (anticipated activation of the pressurizer spray) were defined as *standard PWR applications*. The two core representations were utilized for comparisons of core-wide and hot subchannel analyses. The obtained results for the steady state calculations show that the hot fuel assembly in the FA-by-FA model and the hottest subchannel in the cell-by-cell model are the most limited core regions and have a minimum departure from nucleate boiling ratio (MDNBR). The coolant temperature rise is in an expected range of 40-50 ^{o}C. The observed none zero void fraction is a consequence of the predicted sub-cooled boiling conditions in the most limited core regions. The estimated MDNBR for both cases is greater than the limited value of 1.3 for the used W-3 critical heat flux correlation. The layout-to-layout comparisons are summarized in Tab. 2.

For the pump coast-down transient the ratio of the core inlet flow rate to the average core thermal power has its minimum at the 3rd second of the transient and the most limited core condition was found at that time for both core models. The core-wide and hot subchannel analyses show very similar results. The hottest subchannel has MDNBR of 2.90 against MDNBR of 3.05 for the hot fuel assembly.

For the bank withdrawal at power transient the ratio of the core inlet flow rate to the average core thermal power has its minimum at the 52nd second of the transient. A sharp power decrease of about 60 % occurs after the 52nd second of the transient. In an agreement with the previous comparisons, core-wide and hot subchannel analyses predict similar thermal limits. The hottest subchannel has MDNBR of 2.54 while the hot fuel assembly MDNBR is a 2.67.

The next simulated core transient was the anticipated activation of pressurizer spray accident. During this transient the core average power, inlet coolant temperature and core flow rate, and outlet pressure were varied. At the 150th second transient time, the pressure is reduced up to 40 % of its initial value. Nevertheless that a power decrease starts at the 45th second, the hot fuel assembly (respectively hot subchannel) void fraction and quality continues to increase following the system pressure reduction until the 60th second of transient time, when a significant power drop occurs. The hottest subchannel has MDNBR of 2.28 against MDNBR of 2.38 for the hot fuel assembly.

Table 2: Core-wide to hot subchannel analyses comparisons

Case	Void Fraction, %		MDNBR	
	Core-Wide	Hot Subchannel	Core-Wide	Hot Subchannel
Steady State	4.1	6.8	3.16	3.12
Flow Reduction	17.4	20.8	3.05	2.90
Power Rise	31.7	37.3	2.67	2.54
Pressure Reduction	67.6	71.4	2.38	2.28

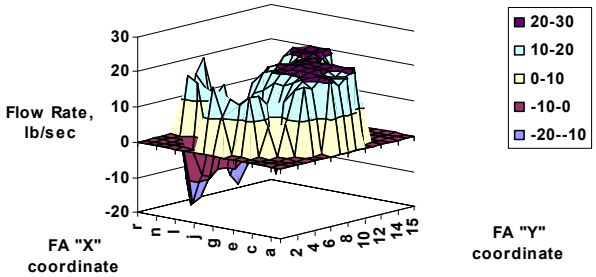
To assess the code capability of simulating negative flow velocities at conditions close to natural circulation, a functionality test with a simplified main steam line break (MSLB) scenario with coolant reduction up to 3 % of the nominal core flow rate was defined as a *PWR challenging application*. To account for asymmetric effects the whole core was modelled where each fuel assembly was represented by a thermo-hydraulic channel. The simulated MSLB transient scenario starts with a pipe break opening between the steam generator and the turbine. The reactor trip occurs approximately 5 seconds later. The real COBRA-TF simulations start after the scram. During the next hundred seconds the system pressure is reduced up to 30 % of its nominal value. Because of the core overcooling a return to power occurs. The main circulation pumps coast down at the 112th second and 50 seconds later the core inlet flow decreases up to 20 % of its initial value. The flow reduction continues up to 3% at the end of the transient. The low pressure signal activates the high pressure injection system. The pressure starts to increase and reaches 80% of its nominal value at the end of the transient. The hot fuel assembly is located at the periphery of the core, at the region connected to the faulted loop. At core flow rate below 5% of the nominal value and 125 MWth core power, the only force working against the gravity is the axial coolant density gradient. Then reverse flow conditions are expected at the less power peaked core regions. Fig. 1 depicts the core mass velocity distribution at axial elevation of 1.83 m (middle of the heated length) at the 300th second of transient time as calculated by COBRA-TF.

The obtained COBRA-TF results demonstrated the code capability of analyzing PWR nominal steady state and transient conditions. Even though the hot subchannel calculations are more conservative and give lower core thermal margins, the results obtained with both methods are similar and do not lead to limiting computing times.

To test the COBRA-TF capability of solving large problems with high mesh complexity a test case was modeled at UPM as part of the code validation program. In this case a subchannel analysis is performed using an embedded mesh of 5×5 quarters of fuel assembly where the one of interest is at the center. From interior to exterior different size lumped channels are modeled until reaching a quarter of fuel assembly. This mesh structure allows a more realistic calculation of the cross-flow effects but creates an additional difficulty for COBRA-TF calculation due to the high number of cells with different size and irregular transverse connections between them. The case was simulated in a flow reduction transient situation converging without convergence problems.

Currently, the code PWR validation program is being extended to simulations of the OECD/NRC Pressurized Water Reactor (PWR) Main Steam Line Break (MSLB) benchmark [16] and the OECD/DOE/CEA VVER-1000 Coolant Transient Benchmark (V1000-CT) benchmark [17] in order to assess the COBRA-TF predictions with more code-to-code and code-to-data comparisons.

Figure 1: Radial Distribution of the Mass Velocity



4. COBRA-TF Based Coupled Code Applications

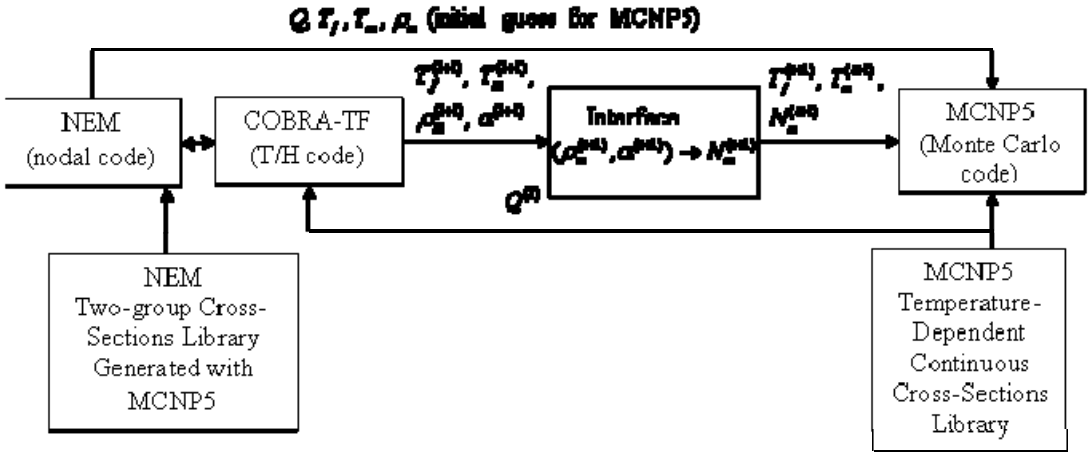
Originally the COBRA-TF computer code was designed to serve as a three-dimensional (3D) reactor vessel model of the COBRA/TRAC thermal-hydraulic code. The stand-alone code version was developed later. However, the use of coupled three-dimensional neutron kinetics/thermal-hydraulics calculations for best-estimate safety evaluation is becoming a common practice. Multi-level coupling methodologies have been already developed at PSU to extend the TRAC-BF1/NEM and TRAC-PF1/NEM computer codes capabilities for evaluation of the BWR and PWR cores local thermal margins utilizing the subchannel modeling features of COBRA-TF [18-19]. In both methodologies the subchannel code was coupled with the pin power reconstruction module of the PSU nodal core simulator NEM. To apply COBRA-TF for hot subchannel/assembly analysis special interfaces were developed providing axial and radial thermo-hydraulic boundary conditions from the TRAC system codes. Time synchronization techniques were implemented for optimizing the multi-level coupling schemes.

As a new COBRA-TF application for coupled calculations a hybrid nodal diffusion/Monte Carlo/thermal-hydraulic code is under development at PSU. The objective of this program is to develop an accurate and efficient methodology for reactor core analysis based on the Monte Carlo method. An innovative acceleration scheme is devised to create hybrid nodal diffusion/Monte Carlo calculations. The nodal diffusion method has currently been the center of the nuclear reactor analysis because of its reasonable accuracy and computational efficiency. However, the present trend in advanced and next generation nuclear reactor core designs is towards increased material heterogeneity and geometry complexity. The continuous energy Monte Carlo method has the capability of modeling such core environments with high accuracy. Because of its statistical nature Monte Carlo core calculations usually involve a considerable computer time to attain reliable converged results for both integral parameters and local distributions. This is especially true when coupling it with a thermal-hydraulics code to obtain 3D power and thermal-hydraulic solutions for a reactor core. The process will be greatly accelerated by calculating the 3D distributions of fission source and thermal-hydraulics parameters with the coupled nodal neutronics (NEM)/thermal-hydraulic (COBRA-TF) code and then using coupled Monte Carlo (MCNP5)/COBRA-TF code to fine tune the results and obtain an increased accuracy. In addition, the computational time is further shortened by performing the MCNP5/COBRA-TF fine tuning calculation in parallel computing environment. The multi-level coupling scheme is shown in Fig. 2. The coupled system will be applied to analyze advanced LWR assembly designs, color-set configurations, and core symmetry sectors.

Another new coupled application of COBRA-TF is being developed at UPM. The coupling will be accomplished at two levels. At coarse mesh level, the code will be coupled with the few-groups nodal diffusion code ANDES [20] that has been developed and it is being tested in the framework of the NURESIM project [21] from the European Commission. This coupling is based in the experience obtained with the coupling of the previous versions of the codes; SIMULA [22], two group nodal diffusion code, and COBRA III [23], subchannel analysis code for homogeneous fluid, that where integrated in one code called SIMTRAN [24]. The second level is fine mesh coupling with the 3D fine mesh few-groups diffusion code COBAYA3. This code is also being developed and tested and is based on a 2D two-groups previous version, COBAYA [22]. Both couplings will be used to obtain detailed parameters distribution at the whole core using a global-local scheme and taking advantage also of the parallelization techniques that are available nowadays. The coupled calculations at both levels will be performed iteratively and the results of each will be used to correct the boundary

conditions at the other level in next iteration. Fine mesh calculation will be performed locally sweeping alternatively assemblies and color sets. The purpose of this scheme is to obtain pin level distributions of variables at reasonable calculation times and avoiding convergence problems.

Figure 2: Multi-level NEM/MCNP5/COBRA-TF coupling scheme



4. Conclusion

Over the last few years PSU in cooperation with AREVA NP GmbH, Germany and the Technical University of Madrid, Spain has been improving and applying the advanced subchannel code COBRA-TF for LWR safety analyses for both stand-alone and coupled code calculations. The code enhancements consist of improving the software quality and computational efficiency, and extending the code modeling capabilities. The COBRA-TF validation and verification program includes BWR phenomenological tests and plant simulations as well [6, 25-26]. An ongoing work is a comprehensive code validation against void distribution and critical power measurements within the framework of the OECD/NRC benchmark based on NUPEC BWR full-size fine-mesh bundle tests (BFBT) [27].

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