STARS

Safety Research in relation to Transient Analysis of the Reactors in Switzerland

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ABSTRACT

The research collaboration with ENSI in the framework of the STARS program was renewed in 2016 with continued emphasis on the development and validation of multi-physics computational schemes for best-estimate plus uncertainty analyses of the Swiss LWRs. The main outcome of the yearly research activities can be summarised as follows.

On the plant behaviour side, the TRACE validation against PKL-3 station-black-out experimental tests was completed, showing a satisfactory performance in most cases although revealing a large sensitivity to the modelling of heat losses. Concerning fuel assembly thermal-hydraulics, the assessment of the sub-channel code COBRA-TF was continued primarily for PWR calculations. In this context, a shift of the CFD activities towards in-core fluid flow analyses was also undertaken with the development of large full bundle models for the PSBT benchmark. With regards to uncertainty analysis, the approach for Bayesian calibration of uncertainties in TRACE physical models was complemented with the development of a simplified surrogate model based on principal component analysis with Gaussian process regression.

For core physics, the assessment of SIMULATE-5 was continued with focus on PWRs and in this context, significant enhancements of critical boron concentration predictions could be achieved for the open MIT BEAVRS benchmark. Concerning CASMO-5, its validation for burnup calculations against PIE data from the Swiss reactors was updated based on the new in-house CMSYS/BOHR methodology for assembly history reconstruction. A significant improvement of the predicted isotopic compositions could be achieved for most nuclides, including isotopes of high relevance for long-term decay heat and neutron emissions. On the transient side, the validation of SIMULATE-3K against SPERT RIA tests with account of nuclear data uncertainties was continued, revealing a tendency for highest uncertainties in predicted transient power and enthalpies at cold start-up conditions and when using SCALE covariance libraries.

Concerning fuel modelling, the development and validation of FALCON base irradiation methodologies was enlarged to modern Swiss PWR fuel designs. Regarding the phenomenology of clad lift-off at high burnup, the FALCON modelling and analyses of Halden over-pressure tests were continued and revealed the potential for significant effects from bonding and fuel cracking/relocation on the fuel thermo-mechanical behaviour, something that is currently not handled by most of the modern fuel performance codes. On the LOCA side, a model for pulverised fuel relocation in the ballooned zone was developed and a first assessment showed that this could, via the substantially increased local temperatures, lead to an earlier clad rupture compared to an analysis with no-relocation or with uniform fuel stack relocation. Finally, for multi-physics, main focus was given to full core LOCA analyses. In this context, the

COBALT methodology for integrated CMSYS/TRACE/FALCON computations was updated for Swiss PWR analyses. Concerning TRACE, a novel approach for the vessel and core nodalization was elaborated such as to allow for an individual modelling of each fuel assembly and with account of cross-flows. Also, a first assessment of the TRACE dynamic gap model was conducted, showing a satisfactory performance in relation to stored energies and transient fuel temperature calculations but not for clad ballooning/rupture estimations

Table 1:
Perspectives 2016

Plant System and Thermal-Hydraulics	Complete Validation of TRACE against PKL-3 Tests
	Conduct First Application of Global Sensitivity Analysis Methods to Validation of TRACE CHF Models against SETs
	Complete Validation of STAR-CCM+ for ROCOM Experiments and Start Assessment for Fuel Bundle Analyses
	Conduct first Development Stage towards Coarse-Mesh CFD Methodology for PWR Fuel Assembly Flow Analyses
	Establishment and Application of UQ Methodology for STAR-CCM+ Analyses of OECD/NEA FLOMIX Benchmark
Core Behaviour and Reactor Physics	Periodic Model Updates and Core Licensing Verifications for all the Swiss Reactors
	Transition and Assessment of Basic CASMO-5/SIMULATE-5 Scheme for the Swiss reactors
	Development and validation of BOHR/CASMO Methodology for Assembly Burnup Calculations
	Start assessment of nTRACER Capabilities towards Time-Dependant Analyses
	Continue SIMULATE-3K Validation with Nuclear Data Uncertainty Quantification for Enlarged set of SPERT RIA Tests
Fuel Modelling and Thermo-Mechanics	Realization and Completion of On-Call on STAV7 Benchmarking for SVEA-96 Optima 2
	Development and Analysis of RIA LS-Test Rods with new FG Trapping BI Methodology
	Assessment of FALCON Clad Hydrogen Uptake Model with Integration of V&V Matrix in FMSYS
	Complete Falcon V.1.3/GRSW-A Coupling along with Verification for Selected Benchmark Cases
Multi-Physics	Realization and Completion of YUMOD-2016 TS3K On-Call
	Development of Methodology for PWR Full Core LOCA Analyses
	Enlarge validation of TS3K for BWR stability Analysis and Launch Refinements towards Non-Uniform Axial Nodalization Scheme
	Start Familiarisation with CASL Solvers and Methods

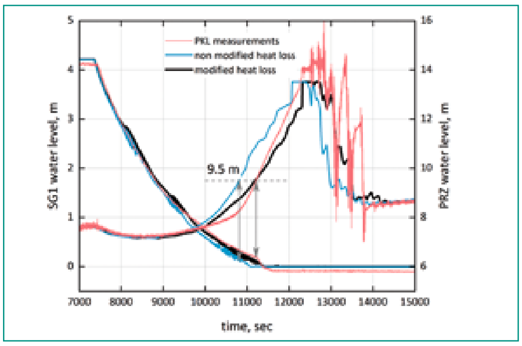


Figure 1:
Effect of Heat Loss Modelling on TRACE Predictions of Water level Evolution for PKL-3 Test H2.2. Run1

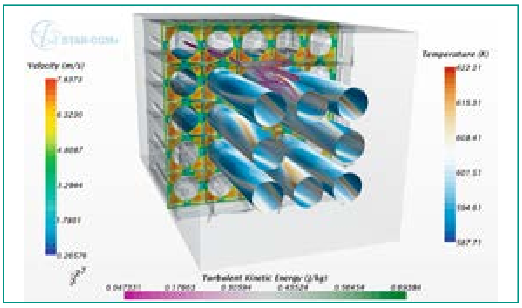


Figure 2:
Star-CCM+ Results for Flow in a full-length PSBT fuel Bundle

Project goals

The STARS collaboration with ENSI aims at scientific support and research related to multi-physics multi-scale modelling and simulations of Light-Water-Reactors (LWR) with emphasis on best-estimate safety analyses with uncertainty quantifications for the Swiss reactors. During 2016, the STARS/ENSI research contract was renewed and the main yearly objectives are listed in Table 1.

Plant system analyses and thermal-hydraulics

The validation of TRACE for experiments in integral test facilities (ITF) was continued during 2016. On the one hand, post-test analyses of OECD/PKL-3 station blackout (SBO) tests (H2.1, H2.2 run1 and H2.2 run2) were conducted. As part of this, the detailed modelling of heat losses from the primary

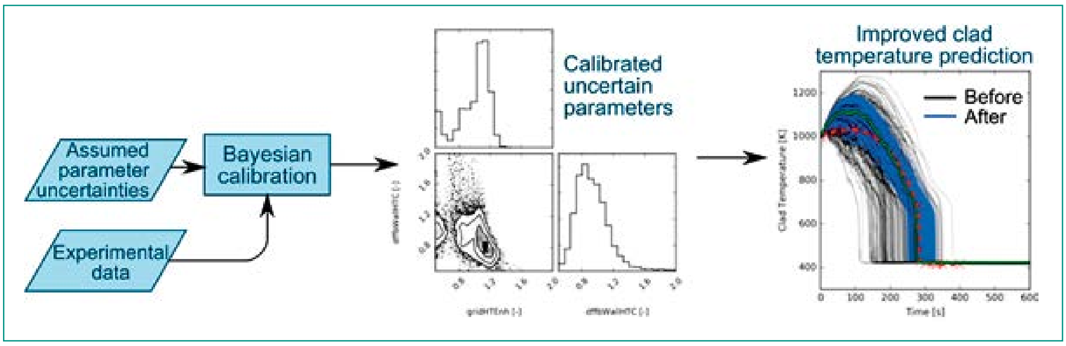


Figure 3:
Bayesian Calibration of TRACE Reflood Model Uncertainties

system components was found to play a key role on the TRACE ability to reproduce the PKL-3 SBO tests. On the other hand, the modelling and analysis of all ROSA/LSTF SBLOCA tests was updated for TRACE v5.0 patch 4 (P4). As part of the update process, several changes were made to the previous RC3 models in order to improve the stability and the quality of results when using P4. Since P4 includes substantial changes in the area of choked flow modelling, the nodalization of the break valves was proven to be the most critical upgrade in all test cases. Regarding separate-effect-tests (SET), the performance of P4 for Pre- and Post-CHF heat transfer analyses was also assessed, showing an overall improvement of the code predictions compared to older code versions. Further assessments for selected boil-off experiments combining both post-CHF heat transfer and boil-off were also conducted, suggesting good TRACE predictive capability at low-flow conditions but not during boil-off where creep flow develops.

Concerning CFD analyses, studies of down comer mixing was continued this year for the ROCOM test facility in the context of the OECD/PKL-2 and PKL-3 projects. PKL-2 test 2.2 and PKL-2 test 2.3 were in this framework simulated using Star-CCM+. At this stage, a clear mismatch between experimentally derived concentration values and the injection tracer was observed and further work will be required to identify the source of discrepancies. For PWR fuel assembly thermal-hydraulics, steps towards using CFD numerical solutions to assess the sub-channel code COBRA-TF (CTF) were also undertaken. Among other things, Star-CCM+ model for a full-length 5x5 fuel assembly from the OECD/NEA PSBT benchmark was developed and steady-state single-phase flow simulations were conducted on 4096 cores at the Swiss National Supercomputing Centre (CSCS), constituting thereby the largest CFD simulation completed in STARS to-date. For a simplified 2x2 bundle geometry without grids, the STAR-CCM+ results were used to assess CTF, showing tendencies of the latter to underestimate the cross-flow between adjacent sub-channels and to strongly over-predict the pressure drop along the bundle. For the latter, studies showed a minor influence from the CTF turbulence mixing model while substantial improvements were achieved with the implementation in CTF of new a wall friction model.

Research on Bayesian calibration of uncertain model and physical parameters in TRACE simulations, using experimental data for the FEBA reflood test facility, was largely completed this year. The calibration, which uses Markov Chain Monte Carlo simulation, has been demonstrated for a 7-parameter FEBA meta-model. The meta-model, a simplified model that accurately reproduces the outputs of the FEBA TRACE model with minimal computational effort, was developed using principal component analysis (PCA) combined with Gaussian Process (GP) regression.

Reactor physics and core analysis

For the CMSYS platform used for steady-state core analyses of Swiss LWRs, an important objective for 2016 was to consolidate the transition from SIMULATE-3 (S3) to SIMULATE-5 (S5). Although less progress than initially planned could be achieved due to a shift in priorities towards BWR dryout, the assessment for PWRs was continued both for the KKG plant and for the open MIT 2-cycle BEAVRS benchmark. For the latter, several model refinements were implemented that allowed to resolve the trend for underpredicted critical boron concentration observed so far. Among other things, it was found that the S5 results would be more sensitive to the reactor operating history, indicating thus the potential to achieve a high performance for the Swiss reactors provided a fine enough burnup condensation scheme is used. And regarding the latter, the in-house BOHR algorithm to reconstruct assembly operating histories (e.g. for downstream FALCON analyses) was enlarged to a coupling with CASMO for 3-D assembly pin-wise nuclide vector reconstruction. Focus was then given to validate this new BOHR/CASMO scheme against PIE data for several Swiss spent fuel samples. And it was shown that through the detailed operating history modelling provided via BOHR, the CASMO nuclide predictions would on an overall basis and for both actinides as well as fission products be significantly enhanced.

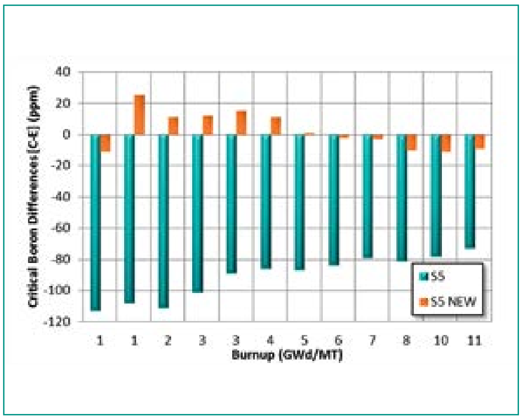


Figure 4:
Assessment of SIMULATE-5 Critical Boron Predictions for PWR BEAVRS Benchmark

Concerning uncertainty analysis, two important milestones were achieved during 2016. On the one hand, a pilot study to integrate nuclear data uncertainty quantification in CMSYS core analyses was completed for a PWR plant, showing significantly lower uncertainties for assembly power distributions than reported so far in the open literature, For transient analyses, the validation of SIMULATE-3K against SPERT RIA experiments with account of nuclear data uncertainties was enlarged to all tests from cold-zero to hot full power conditions and with an assessment of three variance-covariance matrices (VCM). Both total power and reactivity showed a good agreement with the measurements for most tests. The spread of results for different parameters was found to be systematically largest when using SCALE 6.2 VCM library (SCL6.2) and smallest with the ENDF/B-VII.1 VCM library. And when comparing tests results, it was found that the largest uncertainties would be obtained at cold start-up conditions. Nevertheless, a non-zero skewness of the statistical distribution of the predicted time dependent parameters was however obtained, something that might indicate an impact from dynamical phenomena on the nuclear data perturbations that is not yet understood and that will need to be further studied.

Fuel modelling and safety criteria

The FMSYS platform for FALCON base irradiation (BI) methodologies of Swiss fuel designs was further developed during the year. More specifically, models for a modern PWR fuel rod design were integrated in association to a full-core LOCA analysis and to consolidate the BI methodology, a validation of the nodalization as well as the numerical/physical models was conducted on the basis of IAEA FUMEX II experimental cases. In this context, specific attention was given to assess the need to integrate in the BI methodology for the Swiss fuel designs, the detailed time evolution of the axial high energy neutron flux shape as this could affect both oxidation but also clad creep and elongation. At this stage, the results indicate a minor effect for PWRs, implying that using the built-in FALCON models should be sufficient even if this remains to be confirmed by enlarging the validation to other cases.

Property, Unit	PIE	FALCON-PSI
Burnup, MWd/kg	71.5	71.6
Gas pressure, MPa	15.2	14.4
Fission gas release, %	18–20	15.5
Fuel axial elongation, m	7.87E-2	4.95E-2
Clad axial elongation, m	8.75E-2	5.95E-2
Max. oxide thickness, µm	154	157.8

Table 2: *Results for a PWR rod (FUMEX II)*

Concerning high burnup fuel performance, an analysis of several over-pressure «lift-off» tests carried out by the OECD Halden Reactor Project (HRP) was performed using an advanced version of the fuel performance code FALCON coupled with the GRSW-A model for fission gas release and gaseous-bubble swelling developed by PSI. The general goal of these experiments and the corresponding calculations is to identify the governing processes

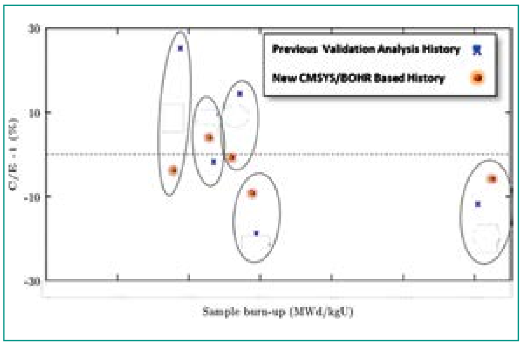


Figure 5:
Validation of BOHR/CASMO against 5 Swiss PIE Samples – Results for ^{244}Cm

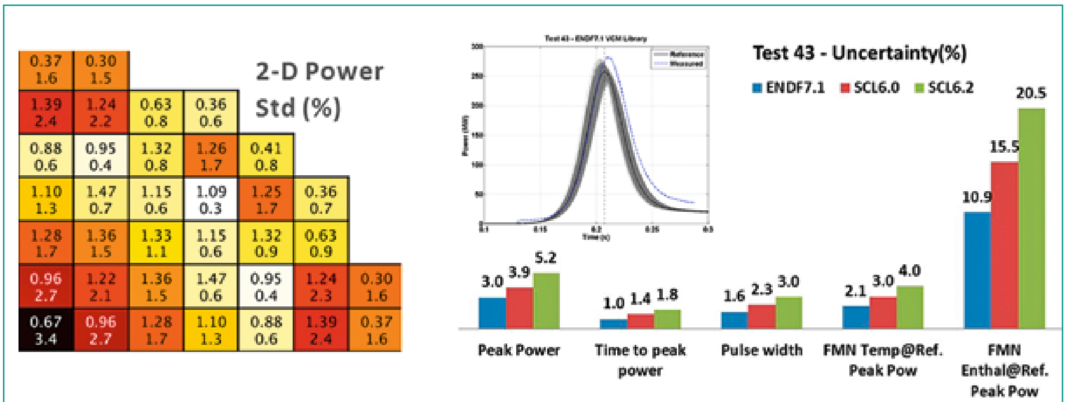
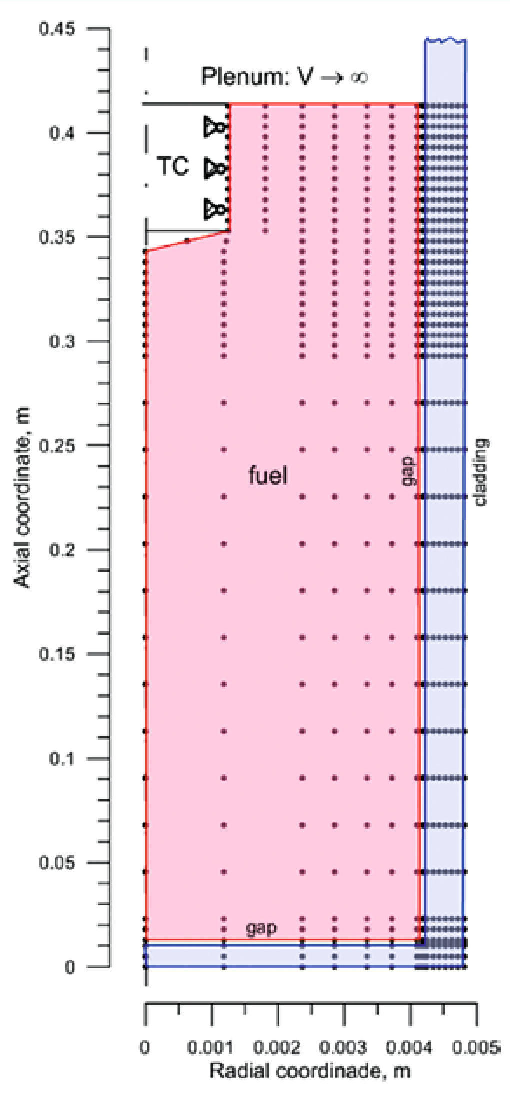


Figure 6:
Left: Uncertainties in CMSYS PWR Assembly Power Distributions due to Nuclear Data (Left) – Right: SIMULATE-3K Analysis of SPERT RIA Test 43 with Nuclear Data Uncertainty Quantification



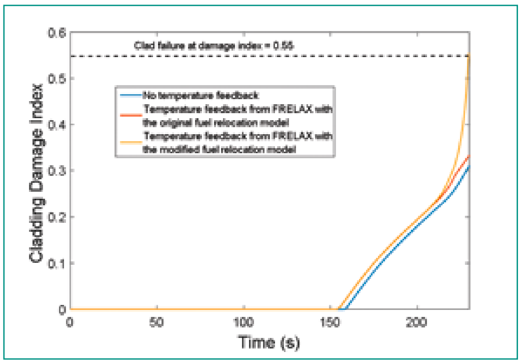


Figure 7: (left) *FALCON Model for Analysis of Halden Clad Lift-off Tests*

Figure 8: (right) *Effect of fuel relocation on clad failure during LOCA Transient*

and specific features of the high-burnup fuel behaviour and, eventually, explore critical conditions for rod failure caused by a very high internal gas pressure. Figure 7 shows the finite-element model applied in the FALCON calculations. Significant effects of bonding and fuel cracking/relocation on the thermal and mechanical behaviour of highly over-pressurized rods, with a fuel burnup of ca. 60 MWd/kgU, have been identified. The effect of bonding is particularly pronounced in the tests with fuel segments pre-irradiated in PWRs. It is concluded, that the identified effects are largely beyond the current state-of-the-art fuel-rod licensing analysis methods.

Finally, with regards to LOCA fuel behaviour, after completion of the fuel fragmentation model, the focus was moved to the development of the corresponding fuel relocation model. As part of this, the cladding damage index for selected Halden LOCA tests was calculated using three different ways: (1) without temperature feedback from FRELAX (no fuel relocation), (2) with uniform fuel stack relocation switch on (original FRELAX relocation model), and (3) the effect of pulverized fuel relocating into the balloon is evaluated (modified relocation model). The key result is the sharp increase in the cladding damage index starting at around 220s. At that time the threshold of 5% for fuel relocation is reached and pulverized fuel starts to relocate downwards. The local temperature increases which leads to a faster damage build-up and, eventually, to an earlier rod rupture. Thus the consideration of pulverized fuel relocation decreases the time to rupture by about 20 seconds compared to no relocation. This is only a qualitative result showing the added value of the modified relocation model, which is relevant only for high burnup fuel where the high burnup structure pulverizes and can easily relocate and thus contribute to the heat source at the balloon. The rupture time is shortened by 9 seconds compared to the uniform relocation model, but the maximum cladding strain is larger.

Multi-physics safety analyses

For multi-physics safety analysis schemes, the validation of TRACE/S3K (TS3K) for BWR stability analyses on the basis of the OECD/NEA Oskarshamn 2 benchmark was enlarged to the blind analysis of stability tests conducted prior and after the event. However, precise measured stability parameters for these tests were not available, preventing thereby to draw any quantitative conclusions on the TS3K validation for these tests even if the obtained results indicate adequate performance from a qualitative point of view. Regarding hot channel/hot rod analyses, the development of a COBALT module to transfer SIMULATE (or S3K) pin power distributions along with assembly inlet/outlet boundary conditions to COBRA-TF sub-channel analyses was started.

As proof-of-principle, test calculations were conducted for a modern BWR fuel assembly design and on this basis, the next steps will be to consoli-

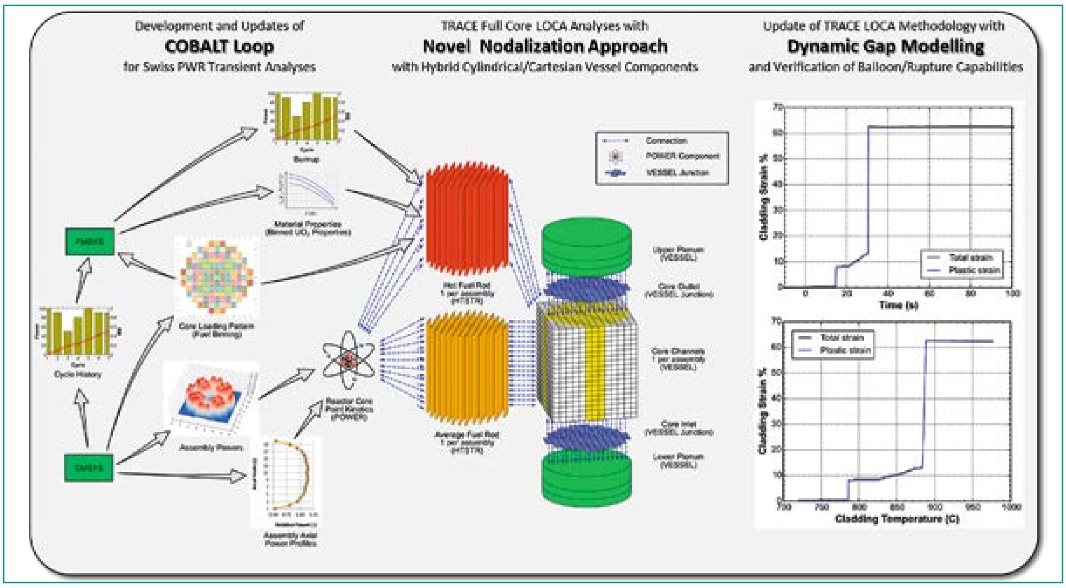


Figure 9: *Multi-Physics Methodology for PWR Full Core LOCA Analysis with Refined TRACE Modelling Approaches*

date this as generalised interface between CMSYS/S3K models and CTF for BWR and PWR hot assembly analyses. Finally, a major part of the multi-physics activities during 2016 were related to full-core LOCA analyses. On the one hand, the studies aimed at core wide estimations of the fuel behaviour during BWR LOCAs (with KKL as situation target) were completed for the reference best-estimate Large Break LOCA (LB-LOCA) scenario, indicating substantial margins to failures because of the relatively mild behaviour of the peak clad temperatures. Further sensitivities are planned to assess the validity of these conclusions for smaller break sizes as well as to identify the level of conservatism needed in the scenario assumptions that could lead to significant rod ballooning and eventually ruptures. On the other hand, an On-Call for PWR LOCA analyses (with KKB as situation target) was launched. To this aim, the COBALT loop for the CMSYS/TRACE/FALCON computational scheme was updated with new modules for PWR analyses. Regarding TRACE, a novel hybrid nodalization approach combining cylindrical and Cartesian vessel components was elaborated in order to allow for full-core assembly-by-assembly representation with cross-flow capability. Regarding the latter, the first assessments for a reference LB-LOCA scenario indicate less conservative peak clad temperature results compared to the multi-channel 3-power zone approach used so far. One reason is the better redistribution of inter-assembly flows leading to less severe voiding and water level reduction in the hot assemblies. Furthermore, the TRACE methodology was also updated with a dynamic gap model, partly to allow for an improved initialisation of the heat structures (i.e. with account of axially-dependent fuel rod characteristics obtained from FALCON) and partly to predict the fuel/clad temperature evolution with account of gap dynamics. To assess this model, comparisons with FALCON were made at the start of the transient, showing consistent axial/radial fuel temperature profiles and providing thus confidence in the predicted initial stored energies. Also, the capabilities offered by the TRACE dynamical model to predict clad ballooning and rupture were evaluated. This showed a non-physical behaviour of the predicted clad strains in the transition between elastic and plastic regimes, indicating that the model is not yet mature and can thus not be applied as simplified alternative to the detailed FALCON fuel rod estimations.

National Cooperation

To complement the research project with ENSI, the STARS program also collaborates with ESB for fuel safety criteria as well as swissnuclear and NAGRA for operational and waste management issues. The project also collaborates with other PSI laboratories as well as with the Swiss federal polytechnic institutes ETHZ/EPFL for the elaboration and supervision of MSc and/or PhD theses as well as for the realisation of courses for the Nuclear Engineering Master Program including «Special Topics in Reactor Physics» and the «Nuclear Computation Laboratory» course on reactor simulations.

International Cooperation

At the international level, STARS collaborates with international organisations (OECD/NEA, IAEA) as part of working/expert groups as well as through international research programs. Also, STARS collaborates with the Finnish regulatory body STUK as well as other technical safety organisations of the ETSON network and with other research organisations. For higher-order core simulations, STARS collaborates with Seoul University (nTRACER) and HZDR (DYN-3D) and during 2016, steps were undertaken to also establish a collaboration with the U.S DOE/CASL consortium in the perspective of further development and validation of the VERA platform. On the fuel modelling side, the collaboration with EPRI as part of the Falcon V1 code development team was continued during the year. Finally, STARS also collaborated in 2016 with E.ON in two main areas, namely CASMO validation for spent fuel characterization and COBRA-TF assessment for PWR analyses.

Assessment 2016 and Perspectives for 2017

During 2016, satisfactory progress was achieved with regards to most of the goals and of particular relevance is that STARS could provide scientific support to ENSI in all its various technical areas. Related to the latter, the research priorities were shifted during the year towards BWR dryout phenomenology and analyses. For this reason, less progress than initially foreseen could be achieved with regards to primarily a) application of global sensitivity analysis methods for validation of TRACE against SETs, b) SIMULATE-5 transition for the Swiss cores; c) validation of FALCON for clad hydrogen uptake. Most of these objectives remain valid for 2017 although high priority will also be assigned to BWR dryout research and analyses.

Publications

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Plant System and Thermal-Hydraulics	Start Validation of TRACE against PKL-4 Tests
	Conduct First Application of GSA to TRACE Validation against SETs
	Validation of COBRA-TF for static and transient dryout tests
	Launch Assessment of STAR-CCM+ for Two-Phase Flow Fuel Bundle Analyses
	Development of Scaled Coolant Mixing Matrices for PWR MSLB Analyses based on STAR-CCM+ ROCOM Validation
Core Behaviour and Reactor Physics	Launch assessment of SIMULATE-5 for BWR Core Analyses with Sub-Bundle Thermal-Hydraulic Modelling
	Complement S3K Validation against SPERT RIA Tests with New CR Adjustment method and Sensitivity Analysis
	Participation to OECD/NEA C5G7-TD with nTRACER code
	Upgrade of SHARK-X Methodology for Uncertainties in Delayed Neutron Data and Kinetic Parameters
	Development and Application of MCNP models for Assessment of CASMO/SIMULATE based R-Factor Methodology
Fuel Modelling and Thermo-Mechanics	Validation of FALCON Clad Oxidation and Hydrogen Uptake Model for Swiss BWR Fuel Rods
	Complete Analysis of RIA LS-Test Rods with new FG Trapping BI Methodology
	Development and Application of FALCON UQ Methodology for WGFS RIA Benchmark Phase 2
Multi-Physics	Consolidation of COBALT.s3COBRA hot-assembly methodology for static/transient CHF analyses in Swiss BWRs
	Development and Application of BWR Bundle TH/FALCON TM scheme for Fuel Rod Analyses under CHF conditions
	Development of OpenFOAM Solver for Coupled Neutronics/Fuel Temperature/Coolant Heat Transfer Analyses in Simplified BWR Geometries

Table 3:
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