ABSTRACT

During 2014, progress was achieved with regards to most of the goals and of particular relevance is that STARS provided scientific support to ENSI in all the various technical areas, including realisation of reload licensing verifications for all the Swiss reactors. On the plant behaviour side, the establishment of a consolidated platform for reference TRACE plant system methodologies along with integrated databases for code/method validation was started. Also, the OpenFOAM solver was introduced for the development of Swiss plant specific models and a first validation of this open source code against real LWR experimental mixing tests was also performed. Regarding core physics, the assessment of SIMULATE-5 for the Swiss reactors and the establishment of nTRACER as next-generation 3-D core simulator were launched. As well, research continued on the development of a hybrid stochastic/deterministic Serpent/SIMULATE code sequence and of pin cell homogenization methods. Also, progress was achieved regarding the validation and/or application of SIMULATE-3K for core dynamics, including an assessment of the code capabilities for critical heat flux calculations during flow transients. For fuel behaviour, efforts were invested towards FALCON/GRSW-A modelling of fuel restructuring effects during high temperature irradiation and to achieve through this, more reliable interpretations of fuel licensing and safety analyses. A consolidation of the FALCON/GRSW-A base irradiation methodology was also launched with the aim at integrating better physical models related to fast neutron flux and to fission gas trapping. On the multiphysics side, first steps towards the COBALT loop aimed at integrating reference plant/core/fuel methodologies with TRACE/S3K transient analyses were undertaken. A new external coupling mode between TRACE and S3K was also developed in order to diversify the core thermal-hydraulics solvers. Regarding uncertainty analysis, the STARS TRACE solution to an OECD/NEA benchmark on LOCA reflood simulations was ranked among the top participants with regards to bounds on experimental data. For nuclear data, the SHARKX methodology was updated with a novel approach to propagate fission yields uncertainties and a first assessment against experimental data was performed. Finally, efforts were continued on the verification of global sensitivity analysis methods to evaluate major contributors to the predicted uncertainty in safety relevant thermomechanical results.
Trace modelling and analyses for the Swiss reactors

During 2014, parallel efforts were conducted in revising the fleet of TRACE models while providing ENSI with scientific support. For KKG, these efforts were focused on setting-up a TRACE methodology for SGTR simulations and analyse on this basis, the plant behaviour including e.g. primary and secondary side coolant releases as function of various pos-
tulated single failures. As part of this, several sensitivity studies were conducted in order to determine the impact from basic analysis assumptions (e.g. pressurizer spray, valve failure, decay heat). Modelling requirements were also investigated, including for instance a study of the SG tube break model (Fig.1, top) in order to evaluate the results without and with account of flow wall friction through the ruptured tube (Model 1 and Model 2 respectively in Fig.1, top). As for the KKL TRACE model, the feedwater system- and the steam line models were both revised. The latter now includes 4 steam lines, bypass and steam header, all explic-
itly modelled. These updates were verified through an assessment of turbine inlet pressure results for a turbine trip test (Fig. 1, bottom). The revised KKL steam line model better captures the very early pressure maxima/minima, compared to plant data. The poorer agreement after 504s hints at errors compensation in the previous model, with a coarser nodalization and an ad-hoc WAZU model resulting in better results.

Assessment and validation of TRACE against STF and ITF experiments

To establish an inventory of «separate-effect» tests analyzed within the STARS project, a scheme was developed to fulfill essentially the following func-

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**Project goals**

The STARS collaboration with ENSI aims at scient-
ific support and research related to multi-physics multi-scale modelling and simulations of Light-Water-Reactors (LWR) with emphasis on best-esti-
mate safety analyses with uncertainty quantifica-
tions for the Swiss reactors. Within this framework, the objectives for 2014 were as follows.
tions: identify the thermal-hydraulics phenomena involved in the performed assessments; provide the data characterizing the code simulations and associated test facilities, develop scripts to execute series of code simulations, automatically covering the array of test facilities of interest, while being amenable to scripting expansion and integration in a broader environment. And in order to meet these objectives, a well-defined information flow sequence was developed (Fig. 2). Essentially, the approach is «phenomena-driven», characterized by the use of double indices to utilize the phenomena interconnectivity. Concomitantly, a simple inventory of the test performed can be obtained at the «Test Facilities» level, and the conducted individual experimental runs can be consulted at the «Experiments» level. The «Input/Output» level is confined to the code files. As an application, experiments used for the post-dryout heat transfer assessment, based on eighteen experiments obtained from four test facilities have been used as testing ground, the results (plots and basic statistics) being automatically compiled in a single document.

Sub-channel analyses

During 2014, the assessment of COBRA-TF for sub-channel analysis was consolidated using OECD/NEA BWR Full-size Fine-mesh Bundle Test (BFBT) boiling tests data (Fig. 3, top). To extract and compare the relevance to void prediction of different model input parameters, a sensitivity analysis was performed using the Morris screening and

![Figure 2: Structure of the TRACE V&V Platform for Separate Effect Tests database](image1.png)

![Figure 3: COBRA-TF void fraction results at exit of the BFBF test bundle Top: Results for 3 selected tests – Bottom: Morris screening for test 4101-58](image2.png)
FAST methods (Fig. 3, bottom). The parameters included boundary conditions (pressure, mass flow rate, power and inlet temperature), geometry (sub-channel area) and code methods (two phase mixing, void drift, heat transfer and interfacial drag).

Among other things, the analysis of the 3 selected tests indicated that the void sensitivity to the selected parameters would differ as function of the location within the heated bundle. More precisely, the void results at the corners for the tests at high pressure (71.6 bar) were found to be very sensitive to the void drift model of the interfacial drag whereas the inner sub-channels were more affected by boundary conditions such as inlet temperature and pressure. The impact of the heat transfer coefficient (nucleate boiling) was also found to vary significantly across the test section.

Development of CFD models for the swiss reactors

Work in 2014 on the CFD modelling of the KKG reactor downcomer and core bypass flows made significant progress towards better understanding the detailed vessel flow behaviour. The model geometry is based on a KKG solid model that was started to be developed in 2013. OpenFOAM was chosen for the CFD analysis because this opens up the possibility for future developments such as one-way or two-way coupling with TRACE. The CFD model will also be used to derive pressure distributions in order to derive relevant mechanical load information or simply calibrate the TRACE model K-factor input parameters. And initial results for nominal operation have already highlighted important phenomena (Fig. 4). For instance, large stagnant recirculation regions in the downcomer have been identified directly below the cold legs. Further, CFD analysis of the core bypass flows has shown that the bypass flow is not fully turbulent, with vortex shedding taking place downstream of the core formers as a result of flow instabilities.

Validation of CFD solvers for high-fidelity safety analyses

During 2014, a validation campaign of STAR-CCM+ was conducted based on experimental measurements performed at the Juliette test facility. The aim was to evaluate the RANS based capabilities to capture coolant mixing distributions in the downcomer and at the core inlet for several loop flow configurations. In Fig. 5, the central plot shows the complete geometry in transparency with streamlines from cold leg 4 (CL4) coloured by the velocity magnitude and also the passive scalar fields in half domain. On the left of Fig. 5, the comparison of the numerical and experimental pressure loads at the upper core barrel is presented. On the right, the distribution of the passive scalar at the core inlet (CI) is shown (tracer injection from CL2). From these analyses, it was found that an appropriate modelling of the swirl at the inlet boundary condition and the turbulent Schmidt number are crucial for accurate predictions. Future developments include the widening of the validation test matrix and the development of an efficient methodology to provide accurate validated mixing matrices at the CI as input for system T-H simulation models.

Core modelling of the Swiss reactor and reload licensing verifications

Taking advantage of the CMSYS platform, STARS conducted for the first time, independent reload licensing verifications for all the Swiss 2014–2015 core designs. These verification analyses were all completed within the limited licensing period and consisted in the development of predictive core models to evaluate safety parameters relevant to both normal operation as well as transients. To
ensure a certain redundancy in the verification results, two lines of models based on CASMO-4 and CASMO-5 were systematically applied. And for one of the reactors, the impact of an intermediate shutdown initially planned for system upgrades was also evaluated. Here, of particular interest was the evolution of nuclides and their impact on the reactivity balance as well as core kinetics parameters during start-up. A nuclear data uncertainty quantification using the SHARKX methodology was integrated as part of this, something constituting thereby a first time application of this methodology for a regulatory support activity. Considering cross-section as well as decay data uncertainties, the estimated uncertainties in specially $^{239}\text{Pu}$ and $^{149}\text{Sm}$ compositions were found to be small (Fig. 6), providing thereby further confidence in the conclusion that the maintenance shutdown would not have any major effect neither at restart nor during the remaining part of cycle operation.

**Hybrid 2-D stochastic/3-D deterministic core analysis methodology**

Considering the advances in Monte-Carlo (MC) methods for LWR applications, one objective of STARS is to evaluate the use of MC codes to generate nuclear data libraries for downstream 3-D core simulators. On this background, the development of a hybrid stochastic lattice / deterministic core two-step sequence based on the Serpent/SIMULATE-3 codes was initiated for BWR analyses. To overcome the high MC computation costs, a simplified case matrix of base depletion and instantaneous feedback branches was first implemented. The predicted reactivity as well as selected few-group nuclear data was then compared to CASMO-5, showing an overall agreement below 1% except for diffusion coefficients. Next, the «SerPl» interface was established to transfer the Serpent 2-D lattice data to SIMULATE-3 (Fig. 7, top) and a verification was conducted for a cycle depletion. Principally, it was found that a reasonable agreement in reactivity could be obtained between Serpent/SIMULATE and CASMO/SIMULATE. The same was found for 3-D power distributions (e.g. Fig. 7, bottom) apart from the core peripheries where differences are most likely related to the diffusion coefficients. However, a non-negligible impact from stochastic uncertainties was observed in the Serpent XS results, prompting the need to carefully study and further optimise the number of histories.

**Higher-order 3-D full core analysis methods**

To achieve higher fidelity 3-D core simulations at the resolution of individual fuel pins, efforts are ongoing for the deployment of higher order core analysis methods. First, the transition to SIMULATE-5 for the Swiss reactors was initiated during 2014. Secondly, the establishment of the nTRACER 3-D pin-by-pin transport code designed for «direct one-step core calculations» was launched. Focus was given to the code scalability on High-Performance-Computers (HPC) for increasingly complex
computational domains. The CPU performance related to each of the main physical/numerical methods was studied in order to identify where a stronger parallelization could reduce the CPU costs (e.g. Fig. 8, left). Third, an intermediate approach based on pin-homogenised solvers is also under investigation. Here, the challenge is to complement the few-group nuclear data libraries with information needed by the 3-D core simulator to handle flux/current discontinuities at the pin-cell interfaces. One approach based on Superhomogenization (SPH) factors was thus established and tested for nTRACER analyses in pin-cell homogenised mode. The SPH algorithm (Fig. 8, top right) was shown to improve significantly the nTRACER accuracy when compared to a CASMO reference solution (Fig. 8, bottom right) but challenges remain especially for the first pin rows of e.g. MOX/UO2 interfaces.

Reactor dynamics and BWR stability
For 3-D reactor core dynamics, the SIMULATE-3K (S3K) coupled neutronics/thermal-hydraulics (T-H) code is the primary solver employed by STARS. During 2014, one main activity was to assess the code capabilities for BWR flow transients (Fig. 9). Using a plenum-to-plenum core model, verifications against separate independent analyses were first carried out, showing a rather satisfactory qualitative as well as quantitative agreement of the predicted core response. On that basis, an in-depth investigation of the transient phenomenology was carried out. Among other things, this showed that the dynamical effects between fuel heat transfer to coolant and void reduction will play a central role for the predicted power response. Thereby, the accuracy will highly depend on the T-H solver capabilities regarding superheated steam generation and dynamical...
momentum effects between the vapour- and liquid phases. Local compressibility effects might also take place which if not properly accounted for by the T-H solver, could lead to a strong under (or over) estimation of the transient power increase rate. Finally, analyses in the entire operating domain showed that the transient evolution would also be highly dependent on the initial steady-state coupled axial power/void distributions.

Another S3K activity was to participate in the OECD/NEA Oskarshamn-2 (O2) international benchmark aimed at a combined feedwater transient and stability event which occurred at the O2 plant. An S3K model was thus developed to analyse Phase-1 of the benchmark and the entire transient including the stability event could be well reproduced (Fig. 10) provided that the recently corrected benchmark specifications on the feedwater temperature were applied. Without activating SCRAM, the PSI S3K analyses indicated a return to a stable state after reaching a maximum power amplitude. As well, the S3K analyses showed that if the feedwater flow and temperature had suddenly been stabilized before SCRAM, the core would have behaved very differently and with a very high sensitivity upon when this stabilization would have occurred. Within a 10-second period, the core could have either continued to oscillate but with much higher amplitude or it could have evolved into a limit cycle, indicating a crossing through a supercritical Hopf bifurcation of the stability boundary.

Fuel restructuring and clad lift-off
A very high-temperature (VHT) irradiation is known to produce a local restructuring of the fuel which eventually results in void formation at the centre of the pellets. The occurrence of such central hole formation is very unlikely in LWRs because of the strict limits on the linear-heat generation rate. Consequently, simulations of these phenomena were so far out of the scope of the STARS fuel behaviour analyses using the FALCON code coupled with the GRSW-A model for gas release and swelling. However, licensing calculations for fuel reliability and safety are usually based on hypothesized challenging operational modes including assumptions on VHT during irradiation. Therefore, to conduct independent verifications of licensing analyses submitted for a new fuel performance code and which included VHT irradiation cases, it was considered necessary to implement a methodology to integrate these fuel restructuring effects in the FALCON/GRSW-A calculations. First, a model to update the finite-element mesh as function of central hole formation was developed. Secondly, a recursive restart technique was implemented to adapt the mesh during irradiation (Fig. 11). On this basis, the impact on important phenomenon such as pellet swelling rate could be studied and a strengthened interpretation of the licensing analysis results regarding e.g. peak fuel temperature or PCMI loadings during ramps, could be achieved. This new fuel restructuring methodology was also used to investigate the licensing criteria applied for clad-lift off related failures.
According to the FALCON/GRSW-A results, it appears that these criteria might be too conservative. More specifically, it was found that the pellet-cladding gap would start growing (Fig. 12) well before onset of cladding failure was indicated by all the available failure-related variables in FALCON such as e.g. the Cumulative Damage Index (CDI). An alternative analysis was performed by imposing a gradual linear increase of the rod internal pressure in the FALCON calculation. With this approach, the condition for cladding failure onset was analytically established and turned out to be as high as ~15 MPa. And this level of pressure difference agrees rather well with experimental findings of a BWR lift-off test carried out at the Halden reactor and with the FALCON/GRSW-A validation results obtained for this test.

Development of models for fragmentation, relocation and dispersal
A PhD thesis aimed at the development of models for Fuel Fragmentation, Relocation and Dispersal (FFRD) during thermal transients and LOCAs is currently on-going within STARS. As part of this, a simplified «gamma transport model» was developed in order to interpret fuel ejection and fuel relocation by considering $^{239}\text{Pu}$ sensitive gamma decaying isotopes found in the spectrum of gamma scans of fuel rods that were subject to LOCA tests at the Halden reactor. Also, emphasis was given to consolidate the FALCON/GRSW-A methodology for base irradiation. First, studies were initiated towards overcoming an eventual limitation in the conventional FALCON calculation approach which relies on a constant ratio between fast and thermal fluxes and which may be inadequate for BWRs because of strong axial void effects. Furthermore and as preparation to a LOCA transient simulation, the development of a model aimed at estimating the amount of trapped fission gas (FG) along the active fuel stack and due to pellet-clad bonding, was launched. The concept is to first calculate the total amount of FG release with FALCON/GRSW-A and to correlate thereafter, the amount of trapped gas and thus released gas to the plenum (Fig. 13) as function of the calculated fuel-clad contact pressure history and total FG release.

Multi-Physics
The coupled TRACE/S3K code system is aimed at being the central pillar for best-estimate multi-physics 3-D core/plant system transient analyses. But its application for the Swiss reactors is challenging not only because of numerical coupling related issues but specially because it requires the integration of robust and rigorously qualified upstream plant/core/fuel methodologies (code, model and physical/numerical methods). During 2014, a new strategy towards this objective was launched among other things in the perspective of full core LOCA analyses. On the one hand, the construction of plant management systems (PMSYS) and fuel management systems (FMSYS) in analogy with the established CMSYS platform were started. For FMSYS, first modules for coupling with CMSYS were developed for FALCON base irradiation based on assembly/pin wise operating history reconstructed from the validated core models. On the other hand, the «COBALT Loop» for integral TS3K analyses was launched (Fig. 14) and the first modules were set-up a) to initialize the TRACE channel- and power components with cycle/burnup and operating point specific core 3-D distributions; b) to set-up the TRACE heat structures with burnup dependent thermo-mechanical data; c) to implement a completely revised steady-state initialization procedure in order to strengthen robustness and convergence of the TRACE models. Regarding TS3K itself, an alternative numerical coupling scheme to the internal coupling mode...
used so far (Fig. 15, left) was developed. With this new coupling scheme, the underlying concept is to use S3K for both core neutronics and thermal-hydraulics while TRACE now handles only the system TH. Through this, one intention is to overcome the necessity to group the core TH channels for long transient simulations or for uncertainty analyses. Another objective is to achieve diversified core TH solvers in order to better understand if the underlying reasons for predicted complex core behavior phenomena could be related to the TH solution scheme. The new scheme developed along these principles (Fig. 15, right) is referred to as external and/or plenum coupling since TRACE and S3K now exchange TH data at the core exit/inlet. However, compared to classical external coupling schemes, a parallel approach was implemented with TRACE maintaining a simplified core TH model in order to ensure TH convergence at the boundaries between core and system. At this stage, preliminary verifications have been made and indicate that the scheme is operational as intended for transients not involving reverse flows. However, no gain in CPU efficiency has been observed and further studies are required to compare in more details both coupling modes for various types of BWR and PWR transients.

Uncertainty and sensitivity analysis
A major activity of STARS is to develop methodologies for uncertainty quantification (UQ) and sensitivity analysis (SA) aimed at multi-physics multi-scale best-estimate safety analyses. Evidently, this requires that such UQ/SA methods be first developed for each technical area, i.e. plant TH, core physics as well as fuel behavior, and this was continued during 2014. Regarding T-H, the UQ study for TRACE simulations of LOCA reflood continued with the completion of the STARS contribution to the PREMIUM benchmark. In this context, the blind-test results from STARS on 6 Pericles reflood tests were ranked with 4 other participants (out
of 17) in the top category «results well bounded». Fig. 16 shows the verification of the Monte-Carlo envelop for the rod temperature of one of the blind-tests, assuming 34 parameters and PDFs selected through in-house expert judgement and preliminarily validation using open data (Feba) from PREMIUM. The main contributors to the UQ were identified by sensitivity analysis using Morris screening: the interfacial drag and wall heat transfer models for dispersed flow film boiling and the spacers heat transfer enhancement model. Finally, Functional Data Analysis (FDA) was employed to extract the first 3 modes accounting for 90% of the variability: the amplitude of the temperature rise (50%), the slope (concavity) of the decreasing phase down to quenching (35%) and the quench temperature (5%).

On the side of nuclear data, a new approach to treat fission yield uncertainties with the CASMO-5 code was developed based on the concept of normalization and respecting physical constraints during the yield perturbation process. Indeed, as two fission product per fission are considered, when a fission yield is perturbed (increased or decreased) another one should be perturbed too (respectively decreased or increased) in order to keep a total of two fission fragments per fission. As well, other constraints like charge and mass conservation have to be fulfilled between the states before the fission process (incident neutron and target nucleus) and after (emitted neutrons and fission products). A methodology using a mathematical projector to add those constraints into the Variance-Covariance Matrix (VCM) has been implemented to the SHARKX tool. To verify this updated methodology, the uncertainties in nuclide compositions due to nuclear data and their various constituents were estimated on the basis of comparisons with experimental data from a Swiss spent fuel sample (Fig. 17). Further assessment is under progress through participation to Phase 2.2 (BWR/PWR fuel assembly depletion) of the OECD/NEA UAM benchmark.

### National Cooperation

To carry out its research and scientific support activities, the STARS project collaborates with ENSI as well as with 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, the project collaborates with international organisations (OECD/NEA, IAEA) as part of working/expert groups as well as through international research programs. The project also collaborates with the Finnish regulatory body STUK as well as other technical safety organisations of the ETSON network and with other research organisations, on the one hand through e.g. the EU 7th FP NU5SAFE project and on the other hand, through bilateral cooperations. During 2014, such bilateral cooperations were established with Seoul National University for the development and validation of the nTRACER code. As well, the STARS project entered a collaboration with EPRI to become part of the Falcon V1 code development team.

Assessment 2014 and Perspectives for 2015

During 2014, 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. However, multi-assembly sub-channel modelling was not started because it was considered of higher priority to consolidate and complement the single-assembly assessments with sensitivity analyses. Also, the intended validation of S3K against RIA experiments could not be launched, partly because higher emphasis was given to operational and flow transient analyses. Finally, due to the the departure of a scientist in the fuel area, the clad oxygen diffusion activities and the further participation to a RIA fuel code benchmark were not started since after replacement, higher priority was given to the consolidation of reference methodologies as well as to the transition to the new Falcon V1 code. As most of these objectives remain valid, the perspectives for 2015 are specified in Table 2.

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Table 2: Perspectives 2015


