

# STARS IV

## Safety Research in relation to Transient Analysis for the Reactors in Switzerland

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### ZUSAMMENFASSUNG

Auf der Basis der Nachrechnung von mehr als 100 kritischen Konfigurationen aus dem «International Handbook of Evaluated Criticality Safety Benchmark Experiments» wurde die rechnerische Marge ermittelt, die bei der Benutzung des Monte-Carlo-Codes MCNXP für die Kritikalitäts-Sicherheitsanalyse angewandt werden muss. Auf dem Weg zu einer modernen PSI-Methodik für die Kritikalitäts-Sicherheitsanalyse stellt dies einen wichtigen Meilenstein dar.

TRACE, der neue Systemcode der US NRC, wurde mit unterschiedlichem Erfolg für verschiedene Studien eingesetzt. Mit der Nachrechnung einer grossen Anzahl von CHF-Experimenten wurden gute Resultate erzielt, wie auch mit der Nachrechnung des LOFT L-2-5 LOCA-Experimentes, das im Rahmen der PSI-Beteiligung im PSI-BEMUSE-Programm erarbeitet wurde. Das verallgemeinerte Strahlungsmodell, eine Voraussetzung für die Analyse der geplanten Halden-LOCA-Experimente mit hochabgebranntem Brennstoff, funktioniert ebenfalls. Hingegen zeigte TRACE noch Probleme in der Anwendung auf Siedewasserreaktoren.

Mit der vergleichenden Analyse von ausgewählten RIA-Experimenten des CABRI-Projektes unter Benutzung der beiden transienten Brennstab-Codes

FALCON und SCANAIR wurde die Fähigkeit zur Analyse des Brennstabverhaltens demonstriert und damit ein weiterer wichtiger Meilenstein erreicht. Die Anwendung von zwei Rechenprogrammen mit unterschiedlichen Modellansätzen erlaubte gleichzeitig die Einschätzung der relativen Wichtigkeit von verschiedenen Phänomenen, beispielsweise derjenigen des Spaltgas induzierten Brennstoffschwellens.

Die Doktorarbeit zur Entwicklung einer nicht-parametrischen Methodik für die Quantifizierung der Unsicherheiten der physikalischen Modelle von Systemcodes machte gute Fortschritte. Für die Experimente aus der STARS-Void-Datenbasis ergab die statistische Auswertung der Differenzen zwischen berechnetem und gemessenem Dampfanteil, dass deren Verteilungsfunktion stark vom Massenfluss abhängt.

Mit der detaillierten Studie zur weit verbreiteten Chen-Korrelation, die den Wärme-Transport bei Bedingungen des gesättigten Siedens beschreibt, konnte deren Anwendungsgrenzen (vor allem im Zusammenhang mit den Systemcodes) klar aufgezeigt werden. Anhand von unabhängigen, bei der Entwicklung der Chen-Korrelation nicht verwendeten Experimenten wurde gleichzeitig die Unsicherheit dieser Korrelation quantifiziert.

## Abstract

The calculational margin to be applied for criticality safety assessment with the continuous-energy Monte-Carlo code MCNXP was determined based on the analysis of more than 100 critical configurations from the International Handbook of Evaluated Criticality Safety Benchmark Experiments, thereby achieving an important step towards a corresponding modern PSI methodology.

The TRACE code developed by the US NRC was applied for a number of different studies with varying degree of success. The assessment against a wide database of CHF experiments yielded reasonably good results. The PSI contribution to the CSNI BEMUSE-program, a study based on the LOFT L-2-5 LOCA-test, also produced good results. Furthermore, the generalized radiation heat transfer model that is a necessity for the successful thermal-hydraulic analysis of the upcoming Halden LOCA-tests was found to be operational in TRACE. On the other hand, TRACE still has deficiencies with BWR-related models.

The comparative analysis for selected RIA-experiments from the CABRI-project with both the FALCON and the SCANAIR codes represent an important milestone: the capability for fuel transient behaviour analysis has been demonstrated. The application to two different analysis codes allows at the same time the appraisal of the significance of important phenomena, viz. transient fission gas induced swelling.

STARS participated successfully in the international transient MOX-benchmark with a CORETRAN-submission.

The PhD study on the development of a non-parametric statistical methodology for the quantification of uncertainties in system code physical models progressed well. The evaluation of the errors between the calculated and the measured void fraction for the tests of the STARS void database revealed different error distributions for different ranges of the mass flux.

The indepth assessment study of the widely applied Chen correlation for saturated boiling heat transfer revealed the limitation of its usage in currentday's system codes and quantified the correlation's uncertainty ba-

sed on a set of very well characterized experimental data that did not form part of the original developmental data set.

## Project Goals

The mission of the STARS project is to maintain and further develop a comprehensive state-of-the-art best-estimate safety analysis methodology – including criticality safety – for reactor states ranging from normal operation to beyond design conditions (before core melt) and integrate the necessary tools into a consistent system. In effect, the STARS project acts as technical support center for LWR Safety Analysis with the following general goals:

- Conduct research necessary to further develop the high level of expertise of the project team as well as to improve the integrated state-of-the-art analysis methodologies;
- Perform independent safety analysis and related studies at the request of HSK;
- Perform studies on safety and operational issues at the request of the Swiss utilities;
- Provide general neutronic analysis incl. scientific services to the Swiss utilities.

Specific goals set for 2004 were:

- Development of a Monte Carlo based methodology for criticality safety assessment using selected configurations described in the International Handbook of Evaluated Criticality Safety Benchmark Experiments.
- Validation and use of Computational Fluid Dynamics for geometries typical of nuclear reactors.
- Completion of BEMUSE Phase II with the ISP-13 Calculations and related TRACE Assessment.
- Analysis of selected CABRI RIA experiments (UO<sub>2</sub> and MOX) using FALCON and ev. SCANAIR for the MOX-cases.
- Participation in the Halden LOCA-experiments with TH and thermo-mechanical analysis.

- Continuation of the research work on uncertainty in the calculation of physics reactor problems.
- Participation in the Balokovo-3 VVER benchmark (OECD/NSC) for validation of the Monte-Carlo based neutron fluence calculations, and first application to KKG.
- Complete analysis of low power and pressure transients using TRACE.
- Evaluate PARCS by performing selected RIA transients.
- Convert a BWR model to TRACE and perform selected plant transients for benchmarking.
- Certification of the Quality Management System.
- Renewal of collaboration contract with HSK.

## Work Carried Out and Results Obtained

Selected highlights from STARS are reported in the following sections and provide an overview of the major part of the STARS work performed during 2004. Some other work will be briefly addressed in the assessment chapter.

### Development of a Monte-Carlo based methodology for criticality safety

Traditionally, criticality safety analysis in STARS has been performed using the deterministic assembly transport code BOXER that was developed at PSI. As the criticality community has since long put strong emphasis on the application of Monte-Carlo codes for this type of safety assessment, developing a Monte-Carlo based methodology for criticality safety assessment has become a necessity for the project. The general-purpose continuous-energy neutral particle transport code MCNPX, the version of MCNP with additional high-energy models, was selected, also considering perceived needs for ADS-related research that lie outside the scope of STARS.

Significant progress has been made in developing a modern methodology for the analysis of compact fuel assembly storage and transport casks. 135 configura-

tions have been selected from the International Handbook of Evaluated Criticality Safety Benchmark Experiments with the following characteristics:

- Square geometry of fuel rod arrays
- Moderation by water
- Moderation ratio:  $1.0 < V_m/V_f < 3.0$
- Fuel rod pitch,  $h < 2$  cm
- Uncertainty of the evaluated experimental  $k_{\text{eff}} < 0.5\%$
- No solid reflectors
- Steel or borated steel as solid absorber – separation material
- Boron as soluble absorber

Calculations with MCNPX (Version 2.4.0) were performed using two continuous-energy neutron cross-section libraries: JEF-2.2 generated by ENEA Bologna and JENDL-3.3 generated by JAERI. Three-dimensional models have been developed for each of the selected configuration, a representative example being shown in Fig. 1.

The goal of this work is to determine the bias of the estimated  $k_{\text{eff}}$  as well as the tolerance interval in order to determine how much margin is needed to ensure that the safety limit is observed for any given configuration. Intermediate evaluations for a subset of the analyzed criticals are shown in Fig. 2 for both libraries. The two sets of results appear to be normally distributed and the two fitted Gaussian distributions show very similar values for the mean and the standard deviation. Currently, work is in progress to study the effect of the choice of the width of the bins on the values of the mean and the standard deviation in order to obtain a robust evaluation.

In parallel, the calculational margin for the deterministic criticality safety analysis using BOXER was updated for three reasons: First, a new version of BOXER was generated after the correction of an error identified recently, and it was also ported to the LINUX operating system. Second, the PSI methodology for criticality safety related BOXER applications has evolved over the years, e.g. 70 energy groups are now regularly used, and third a new statistical treatment of the assessment results more in line with the MCNPX-work has been ap-

plied. A set of critical configurations less comprehensive than the one used for MCNPX was utilized to determine the BOXER-related values for the calculational margin. (This is acceptable because BOXER will in future serve as secondary tool for criticality safety assessment.) When compared to the «original» value assumed in the original PSI-methodology for criticality safety related BOXER applications, a smaller value of the calculational margin resulted from this study.

## Validation and use of computational fluid dynamics

The analysis of single-phase mixing problems in geometries representative of nuclear power plants represents an important goal of STARS. It requires the application of computational fluid dynamics methods that are investigated in the Laboratory for Thermal Hydraulics (LTH) for both single-phase and two-phase applications. The most efficient way for STARS to gain access to these methods is through a collaboration with LTH. Important progress was made during the reporting period.

It represents good practice in STARS to first demonstrate the predictive capability of new methods with their application to adequately documented assessment cases. In the present case, available mixing experiments from a Swedish test facility representing the geometry of the Vattenfall reactor have been selected to evaluate the two computational fluid dynamic codes CFX-4 and CFX-5. This is done with the background of concerns at the international level that have been raised in relation to the credibility of single-phase CFD-applications in complicated reactor geometries.

Computational fluid dynamics codes represent the fluid flow in three dimensions and include models for turbulence. They require a detailed geometrical description of the space accessible to the fluid. Hence, the following aspects need to be addressed and investigated in the present study:

- Construction of the computational mesh;
- Selection and assessment of the turbulence models;
- Specification of inlet and boundary conditions;
- Choice of numerical schemes and convergence criteria.

During the reporting period, a general methodology for input generation for CFD-codes has been developed: It begins with the construction of a three-dimensional model of the Vattenfall reactor based on the Initial Graphics Exchange Specifications (IGES). This specification for the representation of geometrical models is also applied in the domain of Computer-Aided Design (CAD). The IGES-model (shown on the left of Fig. 3) serves as basis for the generation of the three-dimensional computational grid (shown on the right of Fig. 3) using the commercial mesh-generating software GRID-GEN. The significance of this approach lies in the fact that, in future, available CAD-models can easily be converted into computational meshes for CFD-codes with the promise of greatly reducing the effort needed today for the mesh generation process.

First, the consistency of the grid (with a relatively coarse resolution) has been tested and confirmed for one steady-state calculation performed with the CFX-4 code. Sensitivity tests for grids with higher resolution and complexity are on-going.

## Validation of trace CHF and Post-CHF heat transfer models against rit experiments

The new TRACE code is the result of the US NRC plan to consolidate their legacy PWR LOCA-codes RELAP-5 and TRAC-PF1 as well as the BWR LOCA-code TRAC-BF1. STARS decided to explore the capabilities of the new TRACE code (available through the CAMP-agreement between US NRC and PSI) at an early stage with the goal to prepare for a gradual migration of the STARS LOCA-analysis: With first priority, the currently un-maintained TRAC-BF1-code will be replaced with TRACE, and with second priority also RELAP-5 will be substituted. With this background, the assessment and validation of TRACE is an important part of the project activities.

During 2004, the TRACE code was validated against Critical Heat Flux (CHF) and post-CHF heat transfer experiments during the reporting period. The experimental database consisted of a series of experiments that were performed at the Royal Institute of Technology (RIT) in Stockholm, Sweden. Data from single tubes experiments as well as from a limited set of experiments executed in annular test sections, both with inlet sub-cooling close to 10° C, were obtained from

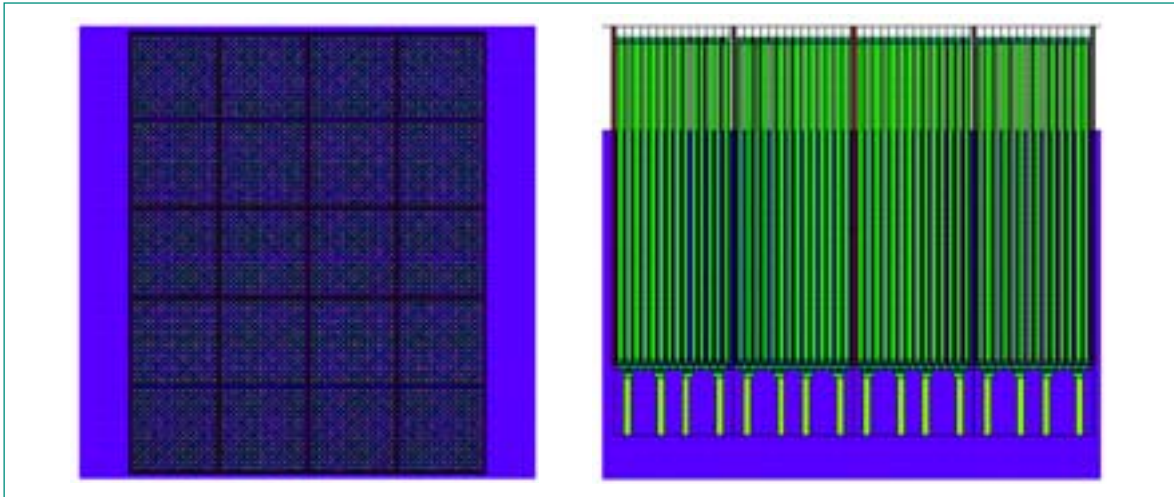


Figure 1: Detailed computational mesh for the MCNPX-analysis of the low-enriched compound thermal benchmark configuration LEU-COMP-THERM-047-01. Left: horizontal view. Right: vertical view.

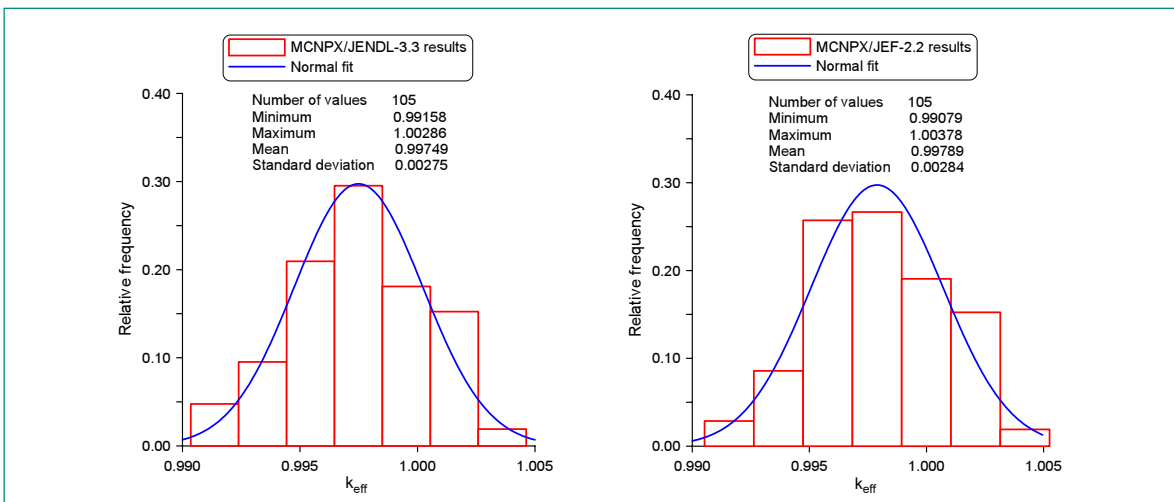


Figure 2: Preliminary results of the statistical evaluation of  $k_{eff}$ -distributions for selected LEU-COMP-THERM configurations. For comparison purposes, a fitted normal distribution is also shown. Left: results using the JEF-2.2 library. Right: results using the JENDL-3.3 library.

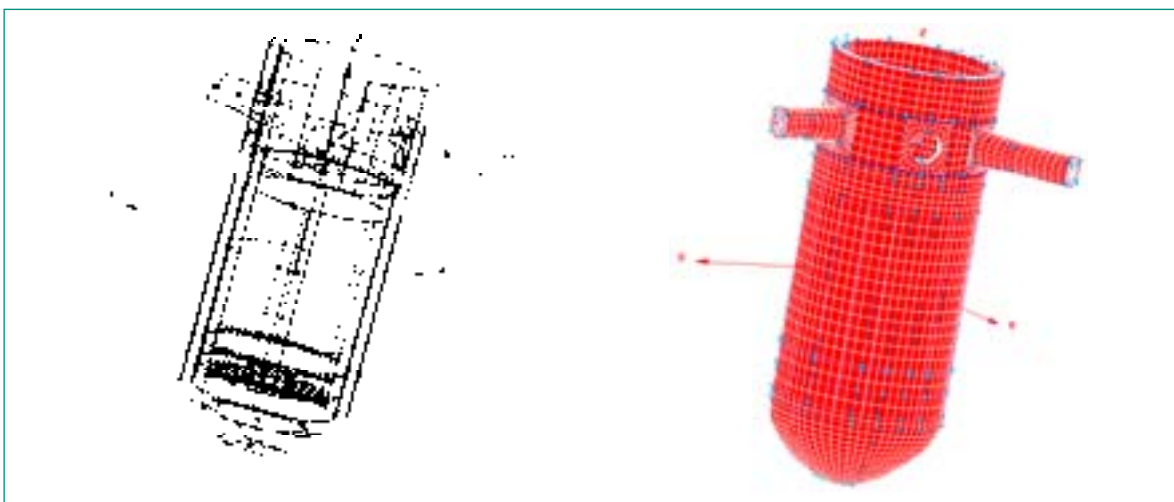


Figure 3: Computational models of the Vattenfall reactor. Left: CAD-like IGES-model. Right: computational mesh generated with GRIDGEN for the CFD-codes CFX-4 and CFX-5.

RIT. The experimental database for single tube geometries covers a broad range of system pressures from 3.0 up to 20.0 MPa and of mass fluxes from 500 up to 3000 kg/m<sup>2</sup>s and it includes tests with uniform axial power distribution as well as non-uniform axial power distributions (featuring power peaking near the inlet, at the middle or near the outlet of the test section). In addition, a limited set of data from experiments with an annular test section and the so-called «double-humped» axial power profile were included in the available data base.

The large database of the experimental data allowed to perform a systematic evaluation of the TRACE code CHF and post-CHF heat transfer models over a large condition range: 131 out of 510 available experiments with single tube geometry and uniform axial power distribution and 328 out of 998 experiments with various non-uniform power profiles were modeled and calculated with TRACE.

Inspection of Fig. 4 shows that the TRACE code is capable of adequately predicting the CHF location for most of the investigated conditions. Poor agreement with the results of the RIT experiments was only found in the low pressure-low mass flux region. The best agreement for the annular tests with the double-humped power profile is found for the low mass flux cases.

However, the TRACE predictions for the post-CHF (in particular film-boiling) region do not agree with the results from the RIT experiments. The current TRACE models representing film-boiling need improvement and additional assessment against a different set of experiments should be performed thereafter.

### **Participation of stars in the Bemuse international programme**

The BEMUSE Programme was started in 2003 with the purpose of performing an international study of the application of different uncertainty methodologies to Best-Estimate system codes. BEMUSE consists of two parts. The first one, which is currently under way and will last until the end of 2005, aims at applying different uncertainty analysis methodologies by a series of organizations (13 to date) for the quantification of the

uncertainties of selected system variables in the simulation of the LOFT L2-5 LOCA Test. The activities involved in this part have been divided into three phases:

Phase 1: organized by CEA-Cadarache (France), involved the description of the uncertainty methodologies to be used and of the characteristics of their application to the uncertainty analysis of system code predictions. This phase has been completed and the report on the activity will be officially released by CSNI. STARS decided to use TRACE as the system code to participate in BEMUSE together with a methodology that propagates input and model uncertainty information to the code predictions through the application of random sampling techniques and non-parametric statistical methods for the analysis of a sample of code output variables. Time dependent and scalar uncertainty measures based in the concept of Tolerance Intervals are used to quantify the uncertainty of the code's predictions. The size of the sample is determined from the Wilks' Formula according to the probability content and degree of confidence assigned to the Tolerance Intervals. This methodology, first introduced at Los Alamos Nat. Lab. by McKay et al., was further developed by Glaesser et al. at the Gesellschaft für Reaktorsicherheit (GRS, Germany) for its use in analyses with system codes, and has been applied in STARS to RETRAN-3D and to the determination of isotopic inventory of highly burnt fuel in depletion calculations with CASMO-4 [1].

Phase 2: consisted in the simulation of the LOFT L2-5 LOCA Test (old International Standard Problem ISP-13) with well-established initial and boundary conditions to be used by all participants. An original L2-5 input deck was modified in order to adapt it to the initial and boundary conditions and made available to the BEMUSE participants by the organizers of Phase 2 (University of Pisa, Italy). The simulation of the L2-5 test with TRACEv4.05 has shown that the code is capable of predicting the main phases of the LOCA transient, including peak clad temperature (PCT), core reflooding and fuel quench, in an acceptable manner (see Fig. 5 *left*) if compared with other system codes used by the BEMUSE participants, e.g. RELAP-5, CATHARE, ATHLET, etc., and with the experimental results. In addition, a series of sensitivity runs, which varied several important system parameters (one at a time) within previously

agreed upon intervals, were also included in Phase 2. The purpose of these calculations was to identify the sensitivity of the code's predictions to these parameters individually, so that this information could then be used in the comparative analysis of the result of the uncertainty calculations in Phase 3. The sensitivity calculations also produced reasonable results if compared to other codes and were completed without lack of convergence, even though the variation ranges considered for some system variables were beyond what should be expected in normal applications for

these kinds of transients (see Fig. 5 right). A report of the results of Phase 2 will be issued also by CSNI in the first half of 2005.

Phase 3: the objective of phase 3, organized by CEA-Grenoble (France), is the application of the uncertainty methodologies described in Phase 1 by each participant to the quantification of the uncertainty in the predictions of PCT and of other system parameters of interest as a function of time. The carrying out of phase 3 in STARS has required the development of a series of in-

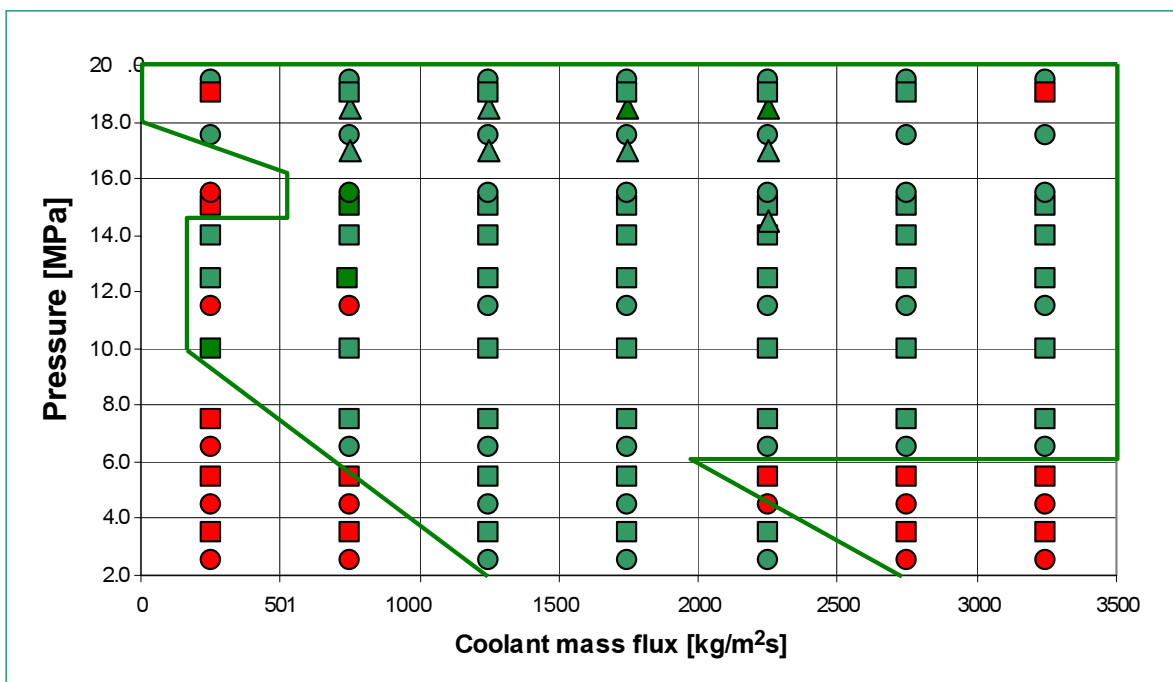


Figure 4: Validity region of the TRACE CHF correlations based on the assessment using the RIT CHF experiments. Green points represent conditions with good TRACE prediction of the CHF location (error in mixture enthalpy is smaller than  $\pm 100$  kJ/kg). Red points represent conditions with poor TRACE prediction of the CHF location (error in mixture enthalpy is larger than  $\pm 100$  kJ/kg).

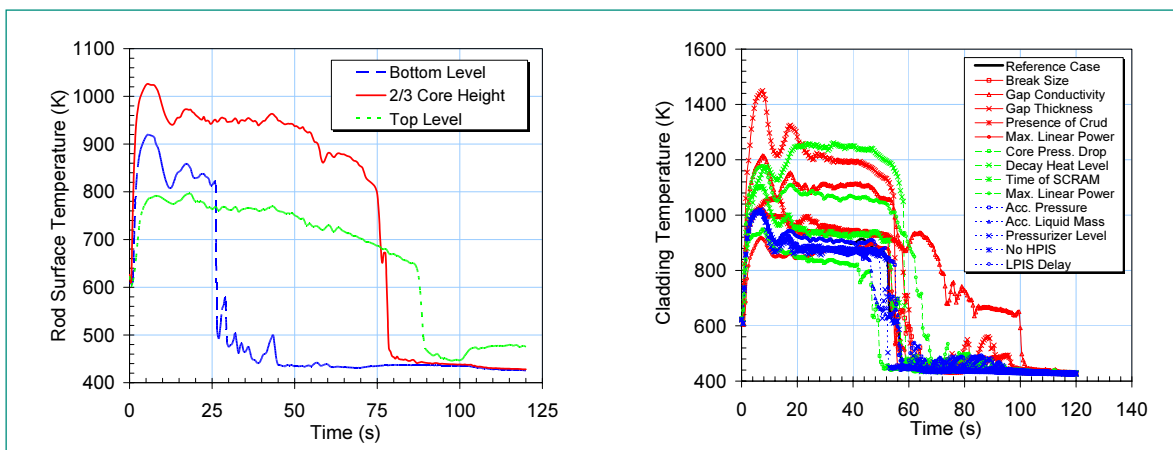


Figure 5: BEMUSE Phase 2 Results of the simulation of the LOFT L2-5 Test with TRACE. Left: Rod surface (cladding surface) temperatures predicted at different axial levels for the hottest rod. Right: Peak clad temperature for the sensitivity runs.

terface programs that link the statistical analysis package SUSAN (developed by GRS) with TRACE. The interface utilizes the information from the sampling process of the input variables and models of interest as generated by using SUSAN sampling algorithms. In this way quantitative uncertainty information is introduced into the TRACE input file and in the TRACE models at run time. TRACE is then automatically executed for the necessary number of times (sample size) according to the probability content and confidence level of the Tolerance Intervals. The collection of the sample values for the system output variables of interest is then achieved by using the AcGrace batch capability linked to an interface code that extracts the information from the XTV files resulting from all the TRACE executions, and then assembles it in a way appropriate for further statistical treatment by SUSAN non-parametric statistical methods. The final result is a series of statistical sensitivity measures and tolerance intervals that quantify the uncertainty in the desired system variables propagated from the uncertainty of input variables and models. This phase is currently active and will be completed by October 2005.

### **Development of a non-parametric statistical methodology for the quantification of uncertainties in system code physical models (PhD Work)**

Doctoral research related to uncertainty analysis in STARS is focused on the development of a non-parametric statistics methodology to quantify the uncertainties in the physical models used by system analysis codes. The research aims at producing uncertainty measures in the form of Probability Density Functions (*PDF*) of the differences between a code model's predictions and experimental separate effect tests. It constitutes a more objective and rigorous approach to code assessment, which yields valuable information for the application of uncertainty propagation methodologies to the analysis of nuclear power plant transients. The work was initiated by assessing the US NRC sponsored system code TRACE for the prediction of void fraction distribution in heated channels. Results from separate effect experiments performed at several facilities (Pericles, TPTF, LSFT, THTF, NEPTUNE, BWR 8 x 8, BWR 4 x 4, etc) were used in order to build a similar void fraction prediction data base to the one compiled for RETRAN-3D in STARS. Analysis of the results

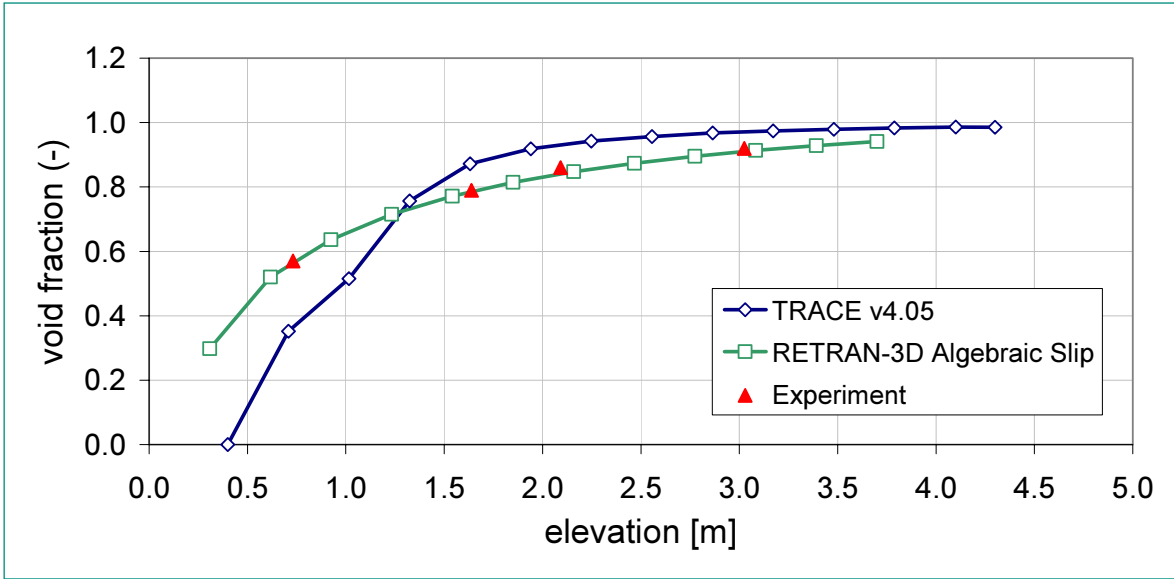
showed that TRACE, in its current version 4.05, suffers from low accuracy in the prediction of interfacial drag at low mass fluxes and relatively low pressures (see Fig. 6). It performs acceptably well, however, for high pressures and mass fluxes representative of BWR operating conditions.

These results suggested using the RETRAN-3D void fraction data base as the data source for the methodology development, which was initiated by developing a procedure based on the *non-parametric universal PDF estimator* proposed by Efromovich. The estimator, based on an optimally truncated and weighted series expansion with a cosine orthonormal base, produces an approximate *PDF* that estimates the unknown probability density function characterizing the distribution of the error  $\epsilon$  in the predictions of a given model. The error has been defined as the difference between the experimental void fraction and the computed one. Considering the entire database available, the values of this quantity constitute a sample and are distributed according to an unknown *PDF*. The methodology being developed also takes into account the influence of independent physical variables on the *PDF*. For instance, when  $\epsilon$  is plotted against mass flux (see Fig. 7 *top left*), one can observe several clusters, which suggests a different *PDF* applicable to different ranges of the variable. As it is shown in Fig. 7, *PDFs* for different ranges of mass flux are clearly different. Future development will define a procedure to introduce this information in the computer code during the application of uncertainty propagation methods to the analysis of nuclear power plant transients.

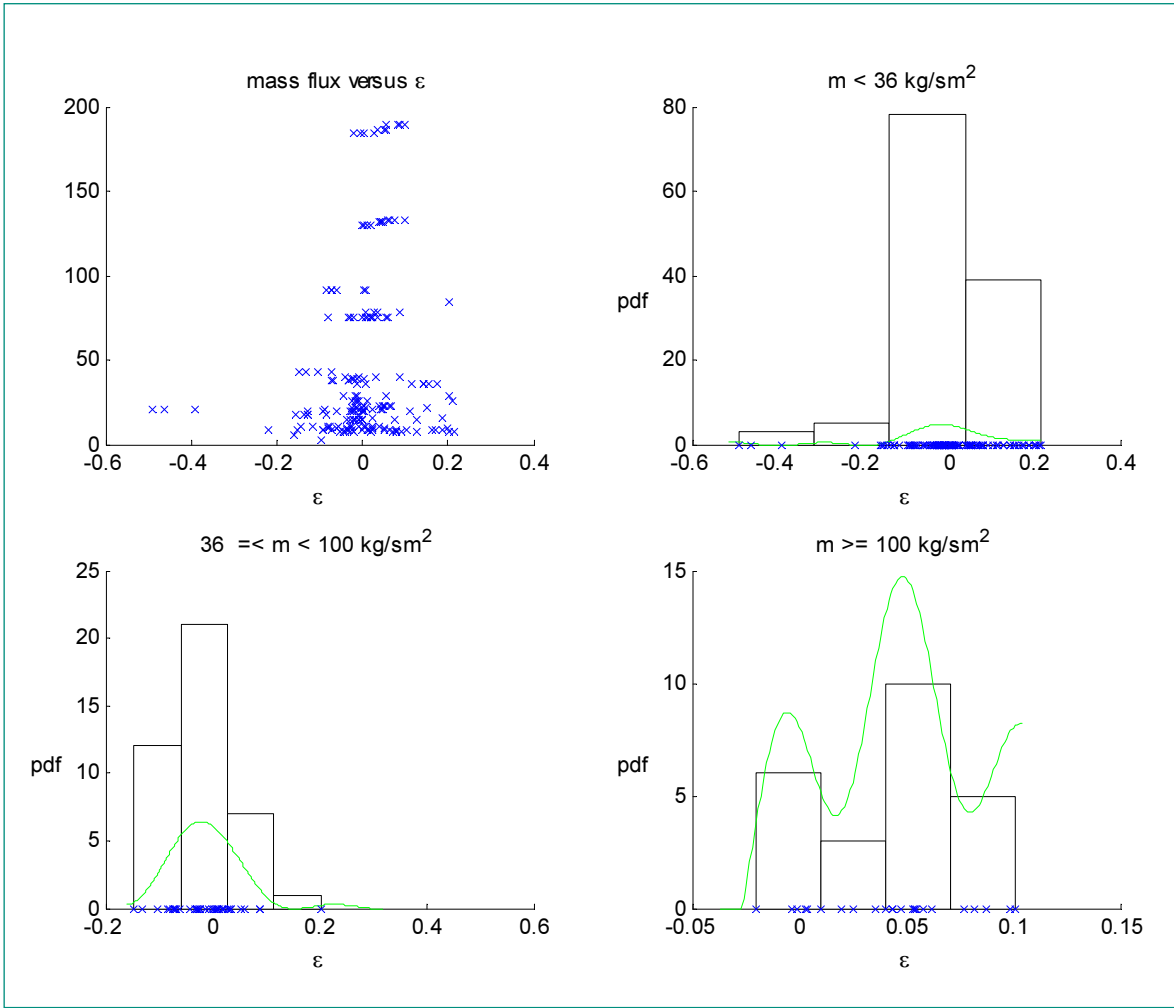
### **Comparing the performance of falcon and scanair against selected cabri REP-NA RIA Experiments**

The transient behaviour of high burnup fuel is investigated for both RIA and LOCA transients within the framework of international experimental research programs. Transferring the results to plant safety analysis calls for analytical tools, viz. transient fuel behaviour codes. In addition, gaining detailed insights into the complex phenomenology of high burnup fuel subjected to transients and, thereafter, building the expertise for transient fuel modelling represent important goals for STARS.





**Figure 6:** Comparison of void fraction profile predictions along a heated tube for one of the TPTF experiments (Test conditions: pressure: 3.05 MPa; mass flux: 130 kg/m<sup>2</sup>s; subcooling: 6 K; heat flux: 128 kW/m<sup>2</sup>). RETRAN-3D with a simple model for the slip velocity based on the drift flux formulation reproduces the experimental values better than the six-equation code TRACE with an interfacial drag model.



**Figure 7:** Distribution of the prediction error in the RETRAN-3D void fraction data base with Mass Flux (top left). PDFs for different ranges of mass flux obtained with the non-parametric estimator based on a cosine-orthonormal base. The different shapes of the void fraction PDF that the model predicts for different mass flux ranges are noticeable.

During the reporting period, emphasis was put on the transient thermo-mechanical analysis of  $\text{UO}_2$ -fuel subjected to fast energy injections as they happen during RIA-scenarios. To this effect, the state-of-the-art fuel behaviour code FALCON – an advanced finite-element based code derived from the FREY code that was used in STARS before – was acquired from EPRI. Through the Swiss participation in the international CABRI-Water-loop project (OECD), the French fuel behaviour code SCANAIR was obtained and it was also included into the mentioned assessment effort.

Selected RIA experiments from the CABRI Rep-Na series for  $\text{UO}_2$  fuel (REP Na-2, REP Na-4, REP Na-5, REP Na-8 and REP Na-10) were used to compare the performance of the two fuel behaviour codes, FALCON and SCANAIR3.2, i.e. their capability to reproduce the experimental results. The study aimed primarily at evaluating the capability of these codes to realistically model fast transients in view of their application in STARS to the determination of fuel safety limits, viz. fuel enthalpy limit in the case of RIA. Hence the investigation focused on the modelling of the mechanical deformation of the cladding and the onset of fuel rod failure.

The analysis of the clad deformation calculated by the codes and the comparison with the experimental measurements show that SCANAIR and FALCON yield different results for the fast pulse tests, e.g. REP Na-2. In fact, while SCANAIR tends to largely overpredict the final clad deformation at the end of the transient, FALCON is shown to slightly underpredict the strain fields generated in the clad, especially at the peak power axial locations. However for the broad pulse cases, e.g. REP Na-4, the codes show good agreement with the experimental results (Fig. 8).

The investigation indicates that the FALCON code reproduces the main thermal-mechanical characteristics of the fuel undergoing an RIA power pulse in close agreement with experiments. The lack of specific models of transient fission gas swelling and release is expected to affect the performance of the code in the form of (a) an underprediction of the state of clad deformation and possibly (b) an incorrect determination of the onset of fuel failure, especially for fast and energetic pulse tests. Power pulse widths for postulated typical LWR RIA events are expected to be  $\sim 20 - 30$  ms (compared to  $< 10$  ms for REP Na-2). It

can thus be speculated that the FALCON code would be able to reproduce the main thermo-mechanical behaviour of the fuel for medium energy injections. However, additional benchmarking is required to fully characterize the potential of FALCON as the main computational tool for fuel safety limit assessment and characterization of fuel thermal-mechanical performance.

### **Mechanical modeling of pressure tube tests using the feat code**

STARS embarked on an exploratory study towards developing a modelling capability for fluid structure interaction. A purely mechanical problem was selected as first study using the multi-purpose finite element code FEAT that is available at PSI through the FAST project: Analysis of the Zircaloy-4 cladding burst tests performed at PSI in the framework of the international NFIR-program (organized by EPRI). These tests have previously been analysed with the fuel-behaviour code FREY.

The cladding burst tests were carried out at ambient temperature. Samples of Zircaloy-4 cladding tubes with different hydrogen content were exposed to a slow internal pressurisation by oil. One-dimensional (radial direction), two-dimensional (axial and radial directions) and three-dimensional FEAT models have been constructed. The results obtained from the FEAT simulations were compared to the data from the burst tests and to the results from the FREY calculations. The sensitivity to the detail of the geometrical modelling was appraised through the evaluation of the results obtained from the three different geometrical models of FEAT. Radial and axial deformations have been analysed, as well as the spatial variation of different stress components, like radial, axial and Hoop stress, the onset of plasticity and the share between elastic and plastic deformations for the results obtained with the three geometrical models. A sample result is given in Fig. 9.

The agreement between the FEAT calculations using the three geometrical models and the experimental data (oil pressure) is very similar to the one between the

FREY calculation and the data. This suggests that more than two-dimensional geometrical models are not needed for the analysis of cladding deformations as experienced during burst tests. From the comparison of the calculated with the measured data it is inferred that the elastic modulus of Zircaloy-4 appears to be ~ 50% higher than the published values, e.g. MATPRO-11, but needs further study.

The capability of the FEAT code for the coupling of elastic/plastic stress analysis with heat transfer and using temperature-dependent parameters was explored, and also scoping calculations for ballooning were performed.

In addition, first calculations for a generic and simple fluid-structure interaction problem have also been started recently.

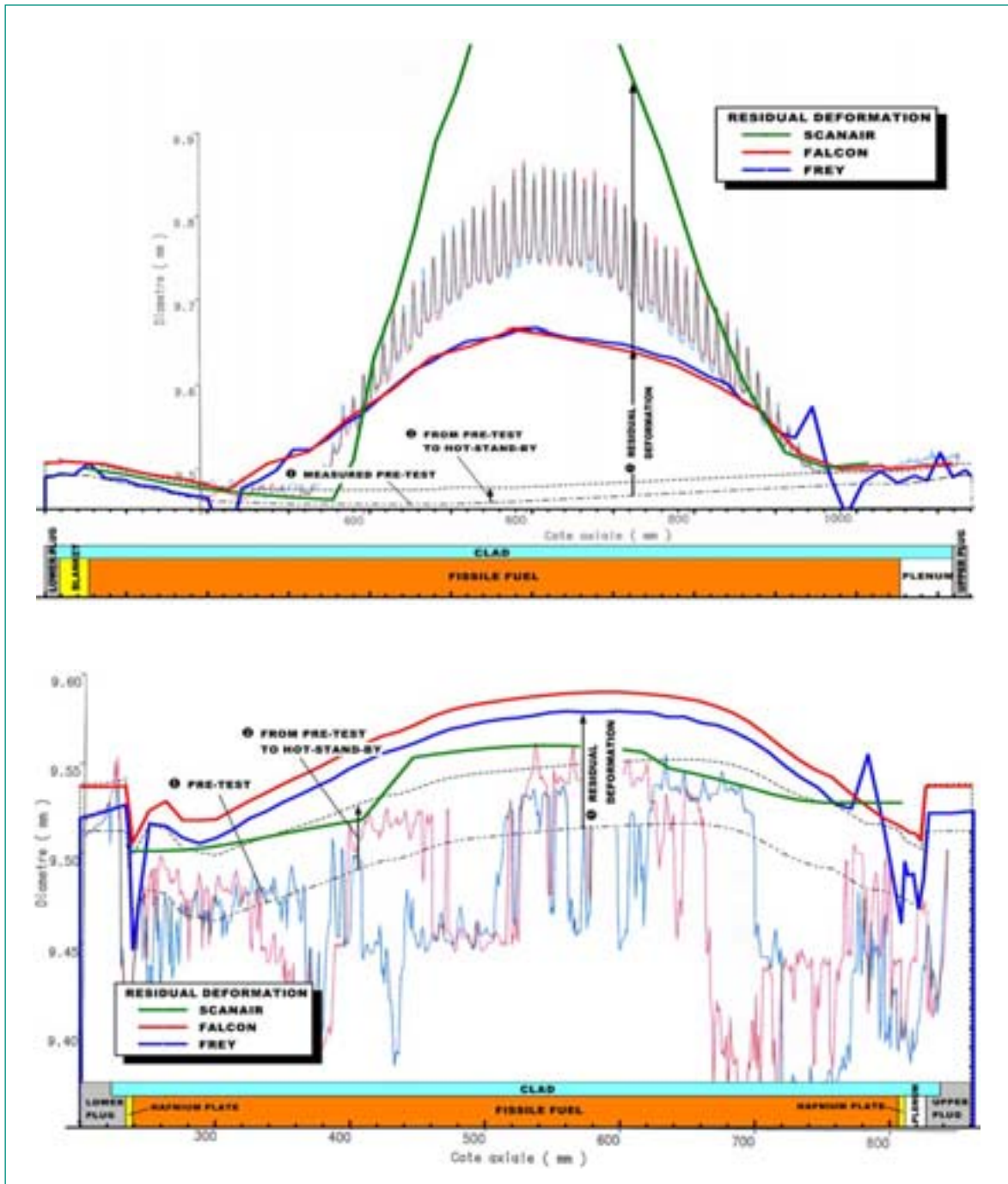


Figure 8: Clad Outer Diameter Profile 10 Seconds after Transient Inception as calculated with the fuel behaviour codes FREY, FALCON and SCANAIR and as measured. Top: Fast pulse test REP Na-2; SCANAIR largely overpredicts the final clad outer diameter profile while FALCON and FREY underpredict the measurement in the peak power axial positions. Bottom: Slow pulse test REP Na-4; the performance of the codes is comparable. (Note that this fuel pin was experiencing extensive spalling.)

## Core Management System CMSYS

The CMSYS system is a Core Management System that has been developed as an integrated computational environment to manage all reactor physics models and corresponding steady-state calculations of the Swiss nuclear reactor cores. The management of the calculations is handled via standardized scripts/programs ensuring that the computations are performed using a consistent, i.e. plant-independent, approach. During 2004, the principal activity has been to consolidate the CMSYS environment in order to enhance the system performance with regards to traceability, security and efficiency. To that aim, a two-level directory structure with regards to access permissions has been integrated. At the first (nominal) level, all the reference (base) models are developed, stored and maintained by the CMSYS administrators. At the second level, non-CMSYS administrators, referred to as external users, can retrieve the reference models and perform specific computations taking full advantage of the CMSYS standardized programs and routines. As a first step toward the implementation of this two level structure, the ATM\_SIM (Automatic Task Module for SIMulate-3) program has been developed to manage SIMULATE-3 calculations. This program not only handles the computations but also ensures traceability (via archiving and storage subroutines), security (by access-checking subroutines) and efficiency (by interface subroutines for external users).

The second main activity for 2004 has been to update the CMSYS models for KKB1, KKL and KKM in compliance with the updated CMSYS structure and to test the ATM\_SIM program. As an illustration, the CMSYS results for the KKM models of cycle 21 to 26 are shown in Fig. 10. The RMS of the deviation between the nodal SIMULATE-3 results and the TIP measurements is averaged over the cycles; shown in Fig. 10 is only the variation around this average. Similarly, the SIMULATE-3 calculated  $k_{\text{eff}}$ -value for local cold critical measurements performed at Beginning-of-Cycle (BOC), is averaged over the cycles and the variation around this average is shown as well. As can be seen, the average TIP difference is below 2% and the variation from cycle to cycle remains within  $\pm 1\%$ , indicating a good accuracy of the computed 3-D power distributions. Concerning the cold critical reference level, reflecting among others the code's ability to predict the passage to criticality in core design studies, the cycle to cycle variation at BOC is within 2.5% (250 pcm), well within the typical licensing range.

## OECD/NEA and US/NRC PWR MOX Benchmark

The accurate prediction of the neutronic response of MOX-cores to localized rapid reactivity injections is highly relevant to STARS because the RIA-related safety limits (fuel enthalpy) for MOX-fuel are lower than the corresponding limits for  $\text{UO}_2$  especially at high burnup. Furthermore, it is well known that no suitable experimental data exist for the qualification of core dynamics codes for RIA-transients. Hence, the STARS participation in the computational benchmark on the analysis of a PWR Rod-Ejection-Accident (REA) transient for a core partially loaded with MOX fuel offered by OECD/NEA and US NRC and hosted by the Purdue University was a natural choice.

STARS participated with its three-dimensional core dynamics code CORETRAN (two-group nodal diffusion). A complete neutronic and thermal-hydraulic CORETRAN model of the PWR benchmark core was set-up in strict compliance with the benchmark specifications. Thereafter, all benchmark cases were analysed using first the standard  $1 \times 1$  neutronic assembly mesh and second the finer  $2 \times 2$  assembly mesh. This allowed to assess the impact of the spatial discretisation scheme onto the analysis of MOX cores.

Although the final benchmark results remain to be published, the PARCS two-group  $2 \times 2$  solution has been made available by the benchmark organisers (Purdue University). An excellent agreement is found between the nodal steady-state solutions produced with CORETRAN and PARCS. The agreement is even excellent at HZP conditions with differences below 1 pcm in terms of both core reactivity and individual rod worths. Moreover, the deviations remain well within 1% in terms of 3-D flux distributions.

The agreement between the transient reactor power predicted by the two codes is also found to be very satisfactory, as shown in Fig. 11: The CORETRAN standard  $1 \times 1$  solution and the PARCS solution match very closely in peak power as well as timing. It can also be seen that the CORETRAN  $2 \times 2$  solution yields the earliest and biggest power maximum,  $\sim 14\%$  larger than both PARCS and the standard CORETRAN solutions. Howev-

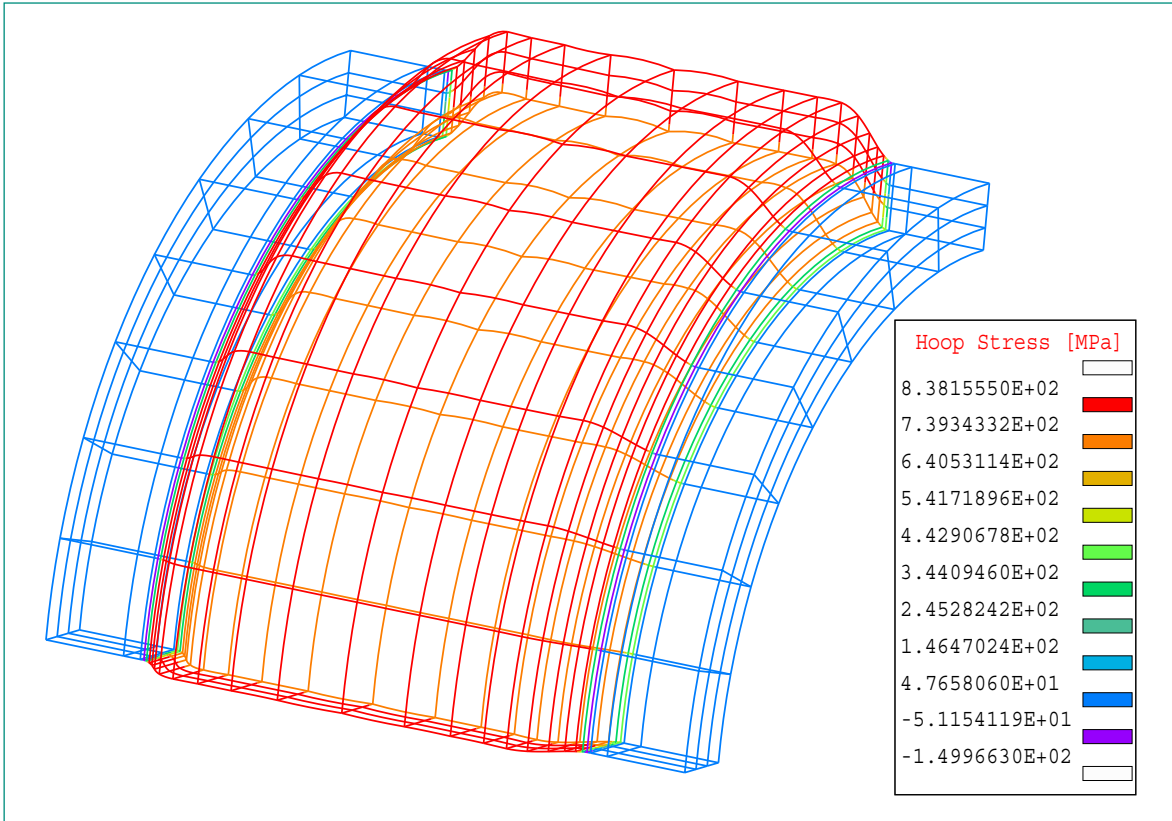


Figure 9: FEAT analysis of NFIR-burst tests. Three-dimensional wire-frame diagram of a quarter of the plastically deformed Zircaloy 4 cladding tube with super-imposed colour-coded Hoop stress [MPa]. The expansion is restricted to the central section since both ends of the tube are tightly fixed. Note: The radial coordinate is magnified by a factor of 20 with respect to the axial coordinate.

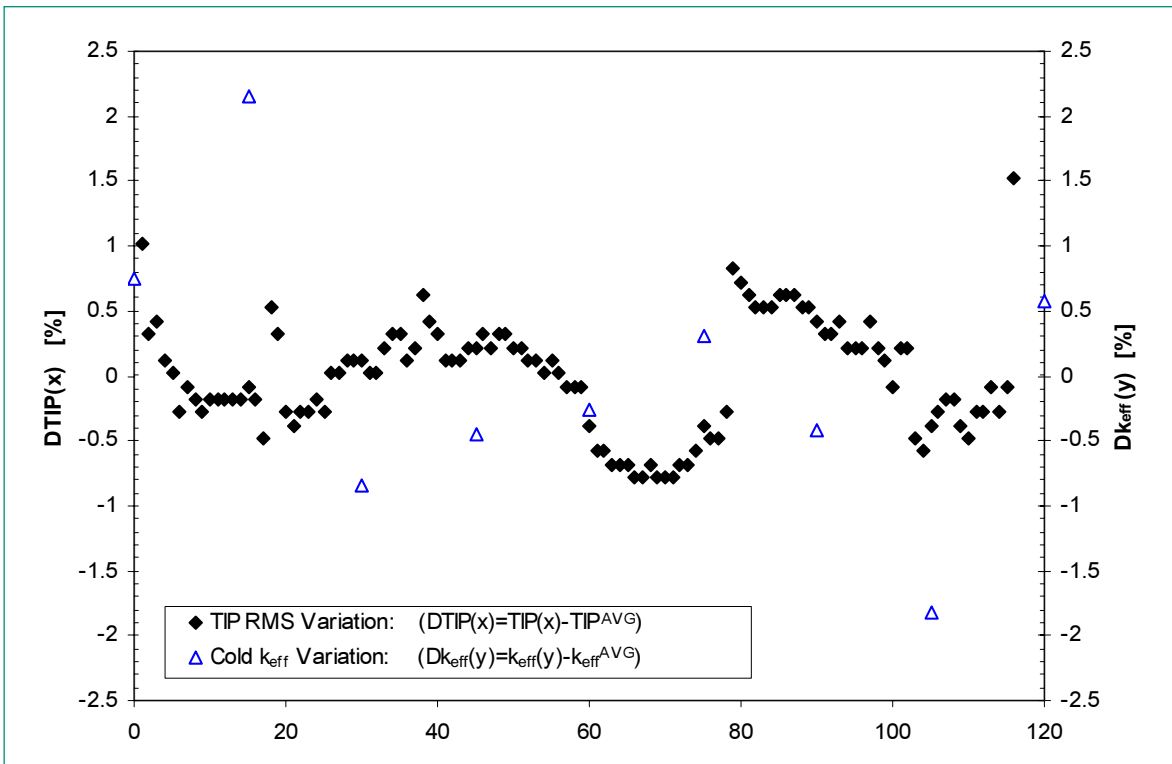


Figure 10: Variation of RMS of difference between CMSYS SIMULATE-3 nodal results and the TIP-measurements obtained for Cycles 21 to 26 of KKM. The RMS averaged over Cycles 21 to 26 ( $TIP^{AVG}$ ) amounts to 1.8% while  $k_{eff}^{AVG} = 0.99298$  for the respective Cold Criticals at BOC. Only the variation around the average RMS is shown.

er, in terms of pulse width and local enthalpy increase, the impact is small indicating that the use of the standard 1 x 1 neutronic mesh for CORETRAN is sufficiently accurate.

Finally, concerning the pin power reconstruction, CORETRAN is found to perform reasonably well when assessed against PARCS since RMS differences well below 5% are obtained. However, a more thorough evaluation will be necessary once the higher-order pin-by-pin transport solution that serves as reference solution of the benchmark will become available.

### The Chen Correlation – a critical analysis

In several best-estimate (BE) thermal-hydraulics (T/H) codes (e.g. TRACE), the standard pre-CHF flow-regime-specific heat transfer correlations (such as those of Thom et al, Jens-Lottes, and Schrock-Grossman) used to construct the so-called «boiling curve»,

have been replaced by a single correlation, the one developed by Chen, originally for the forced convective vaporization mode of heat transfer. Thus, the domain of application of this correlation has been extended to the entire saturated flow boiling and to the subcooled boiling regions, whereas the uncertainty that could entail from this practice has remained essentially uncharted.

While highly accurate boiling heat transfer correlations are not always required in heat-flux-controlled conditions, the need for improved predictive capability for temperature-controlled heat transfer components, such as steam generators in pressurized water reactor (PWR) systems, has been recognized for best-estimate (realistic) calculations.

Thus, this study seeks to address the validity of extending the Chen correlation beyond its developmental database, and splitting the correlation for the development of mechanistic thermal-hydraulics sub-models. This is performed by examining the validity of its consti-

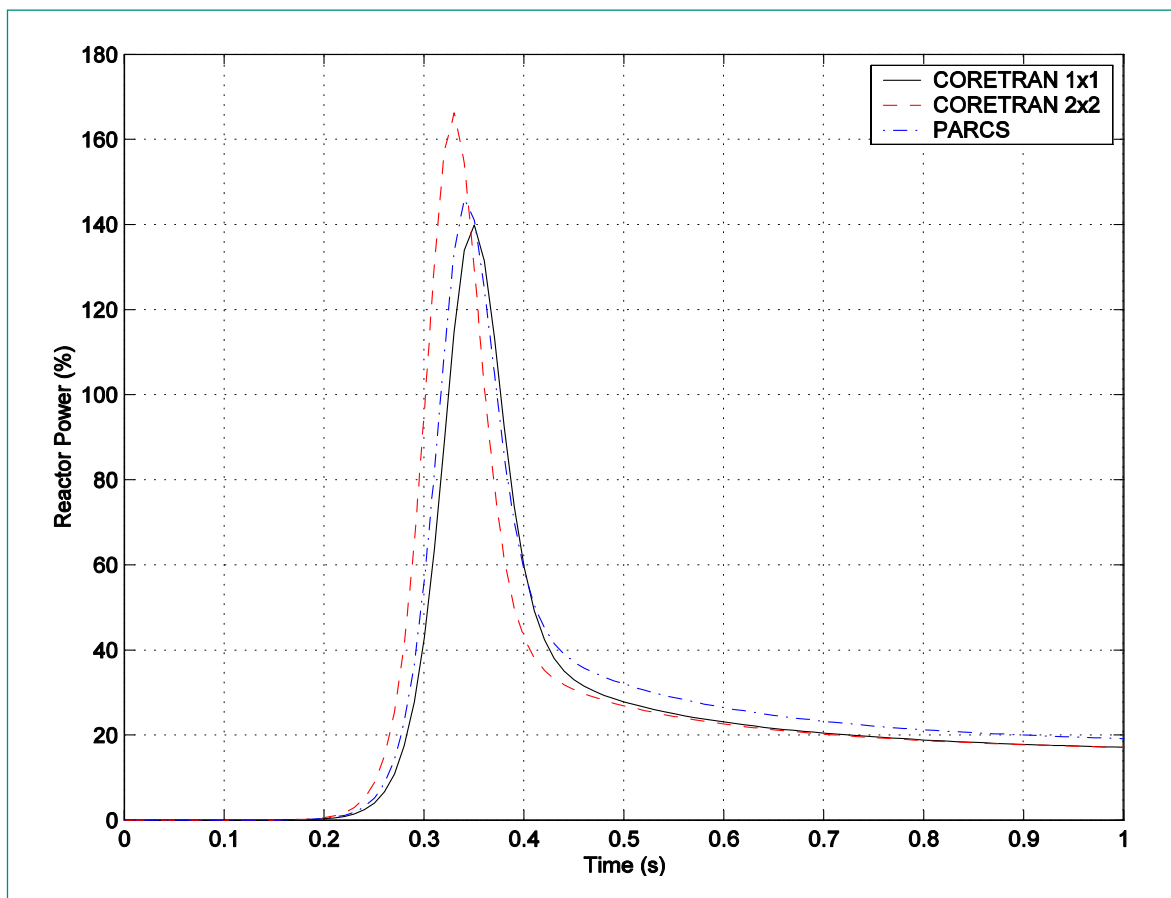


Figure 11: OECD/NEA and US NRC PWR MOX Benchmark. PARCS and CORETRAN results for the evolution of the reactor power. For CORETRAN, two curves are shown representing results from the standard (1 x 1 per assembly) and the finer (2 x 2 per assembly) neutronic mesh.

tuting components, and so individually to remove the risks of compensating errors. The special CISE experiments, performed under BWR flow conditions, whereby the local heat flux and the local quality were decoupled, thus allowing heat transfer data to be measured under *fixed* hydrodynamic conditions, was used for this study [2, 3].

The CISE heat transfer data were analyzed in a separated-effect manner in order to isolate unequivocally the boiling heat transfer contribution. This methodology, possible because heat transfer measurements were obtained under fixed hydrodynamic conditions, yielded several significant results:

1. The measured-to-predicted (M/P) ratio for the prediction of the boiling heat transfer coefficient, when extrapolated outside the range for which it was developed (as done in certain BE T/H codes) was found to vary between 0.9 and 2.9 (see Fig. 12), when the value sometimes assumed for the PDFs vary between 0.8 and 1.2.
2. The boiling component of the correlation was identified to be the root cause of the poor predictive capability of the correlation – when applied outside its original scope. This finding is contrary to published attempts to improve the correlation, where the modification was based on parametric studies to modify the *convective* component.
3. The present identification of the functional relationship for the isolated boiling heat transfer rate provides a new, experimentally-based formulation to modify the Chen correlation. The preliminary tests are good, but the pressure dependence remains to be addressed – although the Chen correlation developmental database covered a system pressures ranging only between 0.1 and 3.5 MPa.

This work demonstrates that in order to *effectively* apprehend the uncertainty associated with a given T/H parameter, carefully selected experiments may be needed to develop *realistic* PDFs, since even for the well-established Chen boiling heat transfer correlation, there is a large discrepancy between the uncertainty obtained from the developmental database, i.e.,  $\pm 11\%$ , and the present results based on a separate-effect approach.

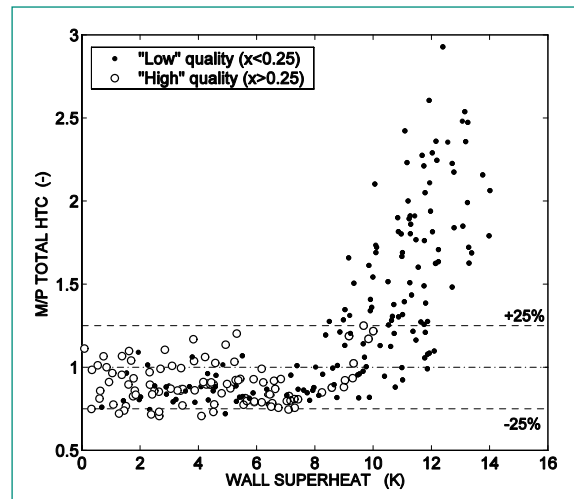


Figure 12: Chen-correlation Measured-to-predicted (M/P) ratio for the total heat transfer in function of the wall superheat.

## National Cooperation

National collaborations are mainly a result of work requested by HSK in the form of contractual agreements called «On-Calls». During 2004, five tasks have been completed, covering the following subjects: Review of a vendor's criticality safety assessment methodology, review of the 3D-kinetics code SIMULATE-3K, representative fuel behaviour analysis and the determination of initial fuel enthalpies to be assumed for MOX RIA-analysis for different plant conditions. In addition, STARS provided technical support to HSK's development of new licensing criteria for high burnup MOX fuel; this included the organization and active participation in a workshop with representatives from the Swiss utilities.

The fruitful collaborations with the Swiss NPPs and with NAGRA continued this year, and several studies were performed: Analysis of the response of the KKL Safety Relief Valve Lines to rapid blow down, Reactor Signal Analysis for BWR Core Stability Evaluation, generation of a new version of the BOXER-MULFIP-code and revision of the validation base for criticality safety assessment using BOXER.

Finally, two doctoral students registered at EPFL's newly created Doctoral Programme in Energy are working on topics related to STARS: One (as already mentioned) is performing research on uncertainty analysis and its application to nuclear safety calculational methods. The second student has started work on improvements for the fission gas modeling at high burnup. These PhD-

studies are performed under the supervision of the head of the Laboratory for Reactor Physics and Systems Behaviour, who is professor at EPFL, with strong support from STARS experts.

## International Cooperation

During 2004, STARS has participated in collaborations with the following institutions:

- Studsvik/Scandpower, Sweden/Norway/USA, which provides maintenance and support for their neutronic codes *CASMO-4*, *SIMULATE-3*.
- Electric Power Research Institute (EPRI), Palo Alto, CA, USA in relation to (a) the maintenance of the system analysis code *RETRAN-3D* (Computer & Simulation Inc., Idaho Falls, ID, USA), and (b) the assessment, maintenance and further development of the fuel behaviour code *FALCON* (Anatech Inc., San Diego, CA, USA). During 2004, several *FALCON* enhancements (mainly utility features) have been developed according to the agreement with EPRI, code assessment being performed using the NFIR-burst tests as well selected Na-cooled RIA-experiments from CABRI.
- Los Alamos National Laboratory (LANL), USA in support of the Monte-Carlo Analyses with *MCNPX* and *MONTEBURNS* (Monte-Carlo with depletion) as one collaborator is member of the BETA-testing team.
- US-NRC through the CAMP-agreement, for TRACE assessment and development. Several code errors have been identified and communicated to the code development team.

As described earlier, in the context of uncertainty analysis applied to thermal-hydraulic calculations, STARS is participating in the CSNI-OECD sponsored **BEMUSE** Programme. During this year, Phase II (of three initial phases) was worked on.

Also as mentioned, STARS participated in the **OECD/NEA – NRC** international PWR MOX benchmark and contributed with *CORETRAN*-analysis.

During 2004, participation in the CSNI task group on the **Action Plan for Safety Margin** (SMAP) continued.

STARS also participated in four international research programs:

First, STARS completed its contribution to the 5<sup>th</sup> Framework EU **NACUSP** project with the submission of the corresponding contribution to the final report.

Second, in the framework of the collaboration with the OECD **HALDEN** Project, the migration of the previously developed TRAC-BF1 model of the test rig dedicated to the LOCA-experiments (IFA-650) to the new TRACE code has started. TRACE features a generalized radiation transport model that is not available with TRAC-BF1; this model allows for the detailed representation of the radiation heat transfer from the hot fuel pin via a heated internal shroud to the «cold» wall of the test rig. The results of the planned LOCA tests with high burnup fuel from the Swiss NPPs are expected to provide further insights into the transient behaviour of high burnup fuel during LOCA-transients.

Third, the collaboration with the OECD **CABRI-Water-loop** Project first provided STARS access to the CABRI RIA-experiments with UO<sub>2</sub>-fuel that are being used for the assessment of the *FALCON* and the *SCANAIR* codes. The latter code has also been obtained from IRSN (F) through this research program. Technical exchange on the modeling of the different experiments is ongoing.

Finally, STARS participated with the TRANSURANUS code using the PSI-fission gas model in the FUMEX-II program that is organized by IAEA [4].

A collaboration with the German research center Rossendorf (**FZR**) was initiated and the topics to be jointly pursued have been agreed upon.

## Assessment 2004 and Perspective for 2005

Most of the goals defined for 2004 could be reached; this year brought again a wide range of scientific services (for both HSK and selected utilities) that put a significant strain on the team, considering that 1 – 2 staff positions remained vacant for a considerable time.

The uncertainty about the future direction of EPRI's maintenance program for *RETRAN-3D*, one of the important STARS transient analysis codes, prompted STARS in 2003 to take an aggressive approach towards implementing the NRC-sponsored general purpose system analysis code TRACE even at the beta-release stage. The



corresponding code assessment effort continued in 2004. While good experience was made for single phase problems with several successful applications, the picture is less positive for two-phase problems despite the reasonably good results for CHF. In fact, the work on shut-down analysis using PKL-data was hindered by code problems and could not advance as planned. The emphasis on the TRACE-work had to be scaled down accordingly and the work of converting the BWR plant inputs to the TRACE format has been postponed.

Also the assessment work using PARCS had to be postponed due to the lack of adequate resources. However, very useful information on the capability of PARCS was gained in the framework of the MOX-benchmark and also through the interaction with our partners at Purdue University.

The work in support of the Halden LOCA-experiments was stopped for a good part of the year, again because adequate resources were not available (the collaborator working with TRAC-BF1 has retired). Work has resumed during the last quarter of 2004.

The presentations by R. Macian et.al. at the PHYSOR-2004 conference found a very positive feedback [5]. This work has been continued with additional cases and will be published shortly.

The work on the Balokovo-3 fluence benchmark did also not progress as planned because this benchmark has not yet been announced officially. In addition, the responsible collaborator was given the task to lecture a reactor physics course at ETHZ. However, the KKG modeling work has started and should yield fluence results around the middle of next year.

As usual, a number of publications appeared that are not directly related to the work of the present year [6-11] but form an important part of the STARS record.

The work towards the certification according to ISO-9001 (2000) of the STARS PMS did not progress as planned during the first half of the year, mainly because the project manager was assigned to lead a task group outside of the project. However, speed was gained during the second half of this year and the team of process responsables has put a very significant effort to interconnect the straight-forward «normal» task processes with the – in the case of STARS – more demanding archiving process in order to

ensure adequate traceability. Certification is now expected at the end of the first quarter of 2005.

For the same reasons, the new contract has not yet been fully developed. However, the presentation of the possible topics as a concept for NewSTARS found the support of the NES research committee.

## Perspectives for 2005

The main items for 2005 are outlined below. Activities in support of the project infrastructure are not mentioned.

- Continue research on uncertainty assessment:
  - Participation in BEMUSE Phase III (uncertainty evaluation for thermal hydraulic problems).
  - Apply methodology to simple reactor physics problem (RIA?).
- Enhance fuel modeling capability:
  - Analyze selected CABRI RIA experiments (UO<sub>2</sub> and MOX) using FALCON and ev. SCANAIR for the MOX-cases.
  - Participation in the Halden LOCA-experiments (IFA-650.3) with TH and thermo-mechanical analysis.
  - Statistical fuel analysis.
- Continue development of Monte Carlo methodology for:
  - Criticality safety and include burnup credit.
  - Neutron fluence calculations for KKG.
  - Explore shielding applications.
- Continue with TRACE assessment (depending on the availability of new code version):
  - Analysis of selected tests from the PKL and ev. the ROSA programs.
  - For BWR applications by converting an existing TRAC-BF1 model to TRACE and benchmarking for selected plant transients.
- Continue development of CFD application for geometries representative of nuclear reactors:

- Analyze mixing experiments in Vattenfalls test facility.
- Apply CFD to lower plenum mixing in the KKG reactor.
- Evaluate enhancements to the core analysis methods:
  - Evaluate PARCS by performing selected RIA transients.
- Initiate active participation in NURESIM (EU 6<sup>th</sup> FW):
  - Explore coupling capabilities of new integrated platform for safety analysis codes.
- Develop a new PhD-topic.

## Publications

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- [4] L. Å. Nordström: **A Mechanistic Fission Gas Model implemented in TRANSURANUS and some FUMEX-II results**, The second Research Co-ordination Meeting of FUMEX-II, Halden (NO), September 7 – 10, 2004.
- [5] R. Macian, M. A. Zimmermann and R. Chawla: **Uncertainty Analysis Applied to Fuel Depletion Calculations**, Proceedings of PHYSOR-4 (CD), Chicago, USA, April 26 – 29, 2004.
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- [7] Y. Aounallah: **Void Fraction and Critical Power Assessment of CORETRAN-01/VIPRE-02**, Nuclear Technology, 145, Feb. 2004.
- [8] W. Barten, P. Coddington: **Peach Bottom BWR Turbine Trip Benchmark Phase 3: Analysis of Full Plant System with 3D-Neutronics using RETRAN-3D**, Jahrestagung Kerntechnik 2004 (M&C 2003 conference, held in Gatlinburg, TN, USA, 6 – 11. April, 2003), on CD-ROM.
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