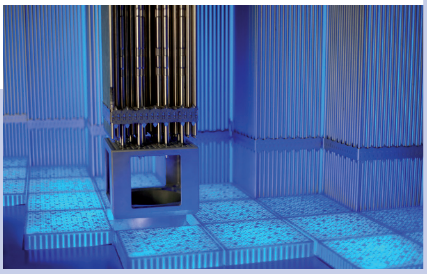
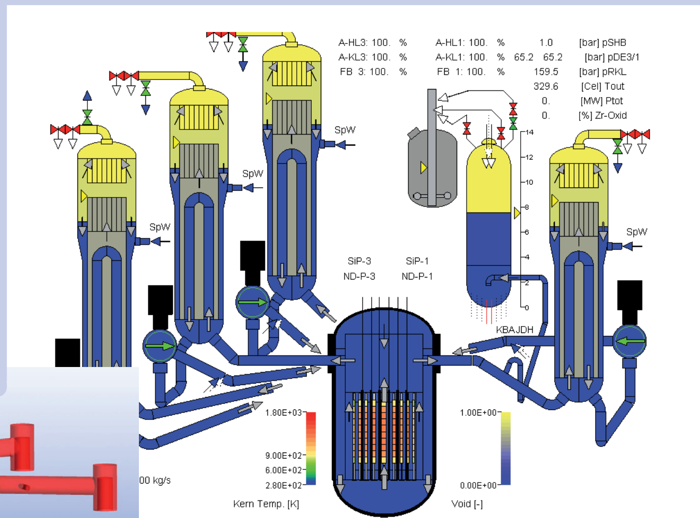
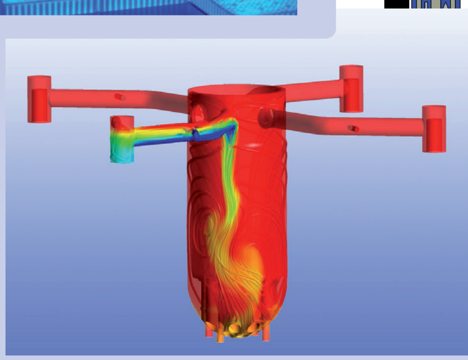
Scientific Codes Developed and Used at GRS

Volume 1
Reactor Safety







GRS - CODES »

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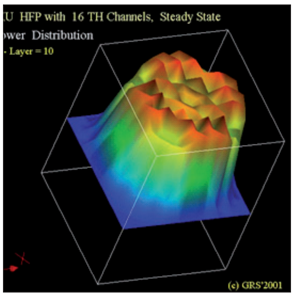
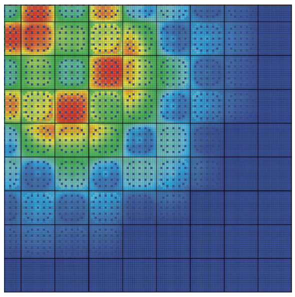
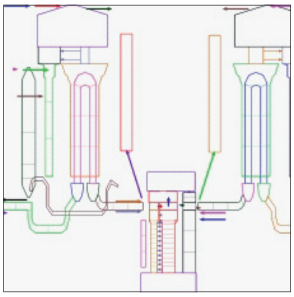
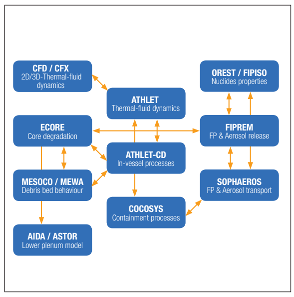
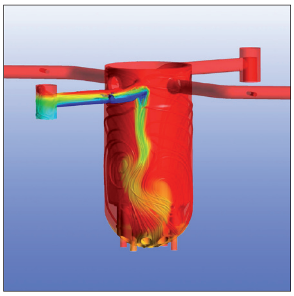
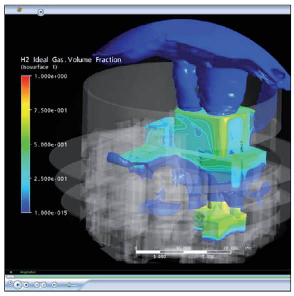


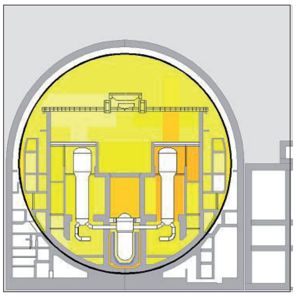


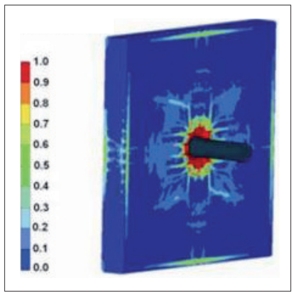


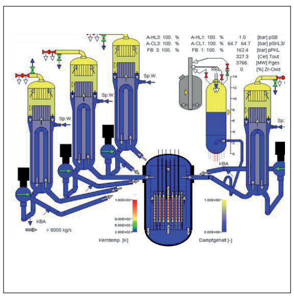


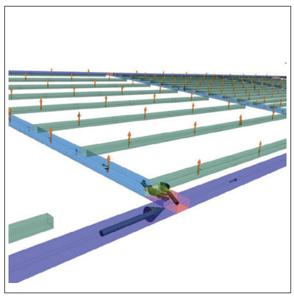












Legend:

– GRS-CODES
– EXTERNAL CODES
– JOINT DEVELOPMENT WITH IRSN

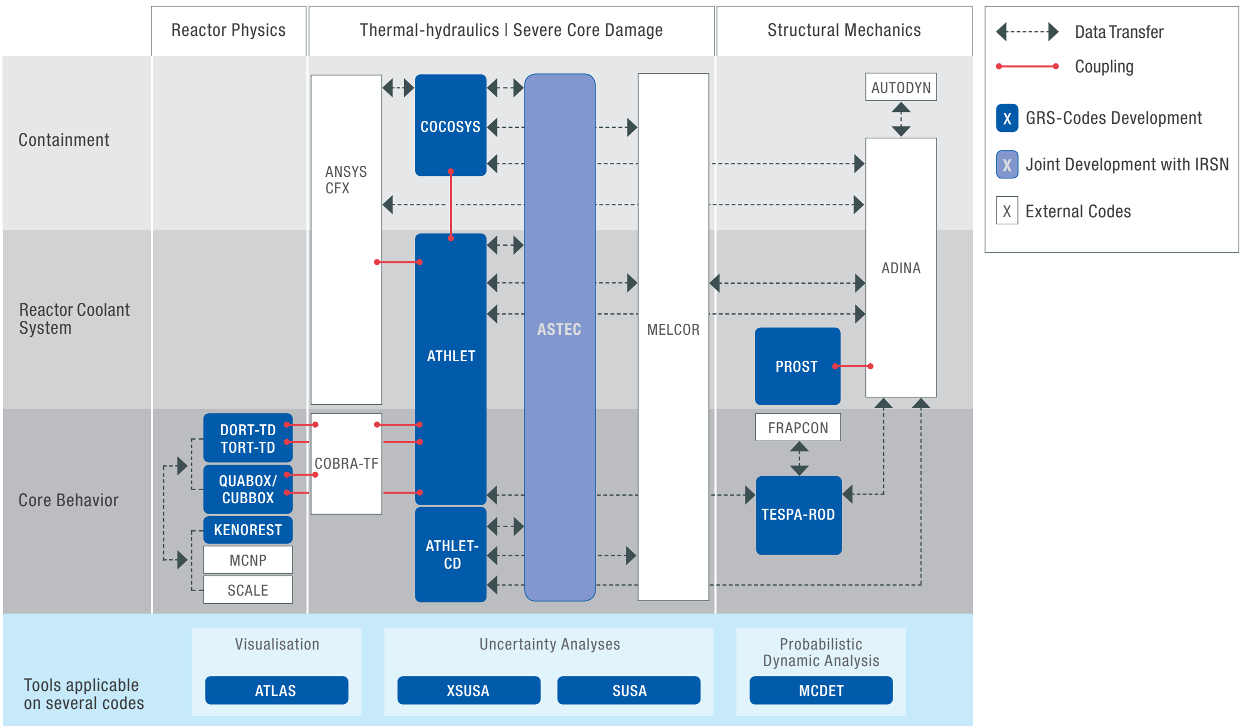
Reactor Safety

The safety analysis for nuclear power plants assesses the performance of the plant against a broad range of operating conditions, postulated initiating events and other circumstances as well as design basis and beyond design basis accidents, in order to obtain a complete understanding of how the plant is expected to perform in these situations and to demonstrate that the plant can be kept within safe operating margins and that accident management measures implemented in the plants are efficient to limit the consequences.

The capability to perform own deterministic analyses for postulated transients and accidents using sophisticated computer models is a key integral part of the function of an independent Nuclear Safety Regulatory Authority for licensing and oversight on the operation of NPPs. To this purpose, GRS as a Technical Safety Organization of the German Authorities is developing, validating and operating a broad range of Simulation Programs for Transient and Accident Analyses in Nuclear Power Plants.

Today, a comprehensive, historically grown code system is available at GRS which consists of own developments and third party codes, many of them coupled with others. The structure of the system is depicted in the figure below.

The codes are split into the fields of reactor physics, thermal-hydraulics and core melt accidents, and structural mechanics. For a complete plant analysis, they comprise containment, reactor cooling system, and reactor core. Some of these codes are integrated in the simulation environment ATLAS for pre-processing, visualization of results and interactive control of the simulation.



Core Behavior

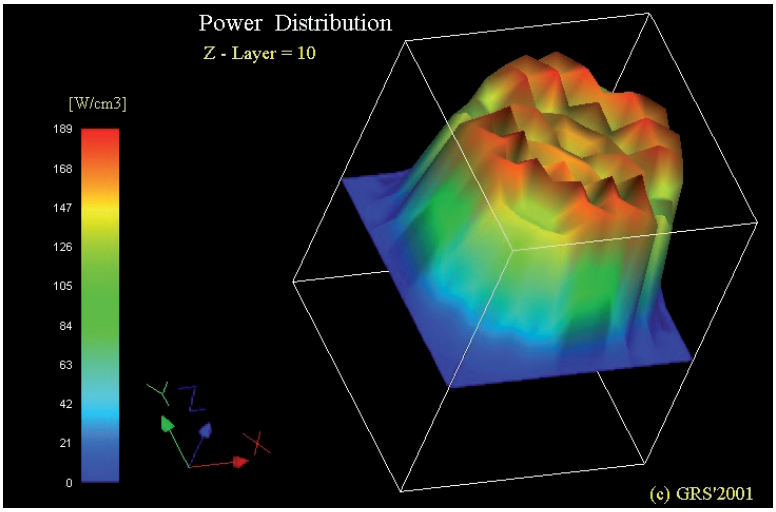
QUABOX / CUBBOX - ATHLET

QUABOX/CUBBOX provides a detailed analysis of the reactor core behavior based on 3D neutronics models which solve the two-energy group neutron diffusion equations including reactivity feedback effects caused by changes of coolant flow conditions and changes of fuel rod temperatures. The efficient solution of spatial and time-dependent neutronics equations is based on coarse mesh methods or nodal expansion methods achieving a high accuracy even for radial nodes corresponding to the fuel assembly size.

The methods deployed in QUABOX/CUBBOX may be characterized by the solution of two-group diffusion equations with six groups of delayed neutrons. The solution method is based on a flux expansion method by local polynomials, enabling to calculate 1D-, 2D- and 3D-core configurations. The code has been developed at GRS for more than 30 years; today it is one of the first nodal diffusion codes with capabilities for assembly-wise and pin-by-pin full core calculations. QUABOX/CUBBOX has been successfully validated at international benchmarks, and is constantly subject to advanced development and validation.

For about 15 years, QUABOX/CUBBOX has been coupled to ATHLET. This coupling allows modeling of the thermal-hydraulic feedbacks. The coupling aims at providing realistic calculations, replacing the conservative model calculations by best estimate calculations; acceptance criteria based on core local parameters can be evaluated more precisely. Application fields of the coupled code systems are e.g. cool-down transients with strongly negative moderator temperature reactivity coefficient in PWR, particularly for high burnup fuel or extended use of MOX fuel; the local boron dilution accident in PWR; ATWS analyses with 3D neutronics models, which reduce the high uncertainties of inherent feedback determining power production and consequently pressure increase.

Today, the coupled code system is the backbone for performing full core production calculations for transient and accident analyses of nuclear power plants with PWR, BWR and RBMK reactors.



Radial power distribution on a horizontal layer in the core - frame from a video

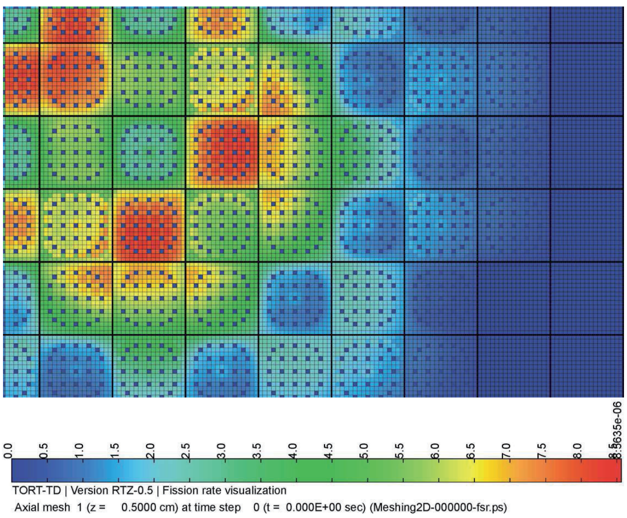
Core Behavior

TORT-TD - ATHLET

The time-dependent 3D fine-mesh few-group discrete ordinates (S_N) neutron transport code TORT-TD is a GRS development for transient 3D core calculations. For thermal-hydraulic feedback, TORT-TD has been coupled with the system code ATHLET, the subchannel code COBRA-TF and the porous medium code ATTICA3D. Whereas the code systems TORT-TD/ATHLET and, in particular, TORT-TD/COBRA-TF is primarily intended to high-fidelity transient fine mesh LWR simulations of both neutron kinetics and thermal-hydraulics phenomena, TORT-TD/ATTICA3D aims at the analysis of 3D issues in high temperature reactors of pebble bed type. The features of TORT-TD include:

- Direct solution of the time-dependent 3D S_N equation for both Cartesian and cylindrical geometry without approximations like, e.g., a quasi-static approach;
- Unconditionally stable implicit time integration;
- 64 bit encoding to meet tight convergence criteria and to enable TORT-TD to be applied to large realistic problems exceeding 32 bit RAM limitations;
- Arbitrary number of prompt and delayed neutron groups; arbitrary Legendre scattering (P_l) and S_N order;
- Fully integrated 3D fine-mesh few-group diffusion solver (steady state and time-dependent) in both Cartesian and cylindrical geometry for fast running scoping calculations to be used as preconditioner for subsequent transport calculations or future embedded transport-diffusion analyses:
- Movements of single control rods or control rod banks;
- Processing of parameterized tabulated cross section libraries for up to 5 state parameters; interpolation either linear or with cubic spline polynomials, thus allowing to study the impact of different interpolation schemes on cross section evaluation;
- Generalized Equivalence Theory (GET) at pin cell level to reduce homogenization errors;
- Time-dependent anisotropic distributed external source capability;
- Leakage and buckling calculation over larger spatial regions (e.g. spectral zones) using the neutron current density in discrete ordinates representation;
- Calculation of Xenon/Iodine equilibrium and transient distribution as a prerequisite for operational transients;
- Graphical pre- and post-processing tools for visualization of input data and output quantities.

Within the applied internal coupling approach, the respective thermal-hydraulic code models the entire fluid dynamics and heat transfer processes in the primary circuit including the core region. The exchange of spatial distributions (power density, thermal-hydraulic state) is managed by interface routines, e.g. the standard ATHLET interface. This allows maintaining each code individually whilst the coupled code is represented by a single executable.



COBRA-TF

The COBRA-TF (**CO**olant **B**oiling in **R**od **A**rrays – **T**wo **F**luid) computer program is a thermal-hydraulic subchannel code initially developed at the Pacific Northwest Laboratory under the sponsorship of the United States Nuclear Regulatory Commission (US-NRC) in order to simulate LWR anticipated transients. Over the last several years, the theoretical models, numerics and computational efficiency of COBRA-TF have been improved at Pennsylvania State University (PSU) and the code has been subject to extensive verification and validation efforts. This advanced version of the code was implemented in GRS in 2008. COBRA-TF solves the two-fluid, three-field equations for two-phase flows in the reactor vessel. For full core calculations, the subchannel formulation (2D: vertical and transverse) is used. The total transverse flow (or cross-flow) between two adjacent subchannels is calculated as a sum of the diversion cross-flows due to lateral pressure gradients and the lateral flow due to turbulent mixing and void drift. COBRA-TF allows very flexible/variable mesh sizes in radial direction (from pinwise to assemblywise resolution) and in axial direction.

TESPA-ROD

The TESPA-ROD (**TE**mperature and **S**train **P**robabilistic **A**nalysis of a Fuel **ROD**) computer code simulates the strain and burst behavior of a fuel rod under the conditions of a loss of coolant accident (LOCA) and of a reactivity initiated accident (RIA) and serves to determine the extent of damage in the reactor core for deriving the radiological consequences of the accident.

LOCA

Since the end of the 90s, Argonne National Laboratory (ANL - USA) has been performing analyses on the different cladding materials under various irradiation conditions. These analyses address the phenomenology of the loss of coolant accident. In parallel, experiments were performed on the behavior of high burn-up fuel under LOCA conditions within the framework of the HALDEN Reactor Project (Norway). The experimental findings have been evaluated and, where possible, implemented in the model approaches for the TESPA-ROD code.

In particular, these recent studies served to further develop the model approaches for the calculation of the hydrogen and oxygen up-take. Further, a model approach to describe the axial fuel relocation in a strained fuel rod due to internal fuel rod pressure has been tested. The modelling of hydrogen and oxygen up-take provided now in TESPA-ROD established the prerequisite for assessing cladding embrittlement as a result of the temperature excursion in steam atmosphere. This means that in future it will also be possible to perform hot channel analyses in addition to damage extent analyses.

Newer reactor core loadings are designed increasingly heterogeneously. This implies the need to consider the fuel rod parameter related to the individual fuel rod in a core damage extent analysis in greater detail than before. By coupling TESPA-ROD with the fuel rod code FRAPCON-2 and -3, a developmental step has been completed which now allows to determine the burn-up history of each fuel rod and thus the impact of this history on the internal pressure and the fission gas composition. Thus, the calculation of the fuel rod parameters, only related to burn-up so far, is extended by a more detailed fuel rod calculation.

RIA

As part of the CABRI test programme, 12 RIA tests have been carried out over the past years. To date, all CABRI tests have been carried out in a sodium-cooled fuel rod environment. After extensive modifications of the research reactor, the next CABRI tests will be performed in a water-cooled fuel rod environment.

All the studies on the reactivity accident (RIA) in the CABRI test facility and the studies in other test facilities

Core Behavior

» TESPA-ROD

(NSRF, BIGR, etc.) show tendencies that increased burn-up reduces the mechanical damage threshold. The evaluation of the CABRI tests shows that at very high power densities in the fuel the strain behavior of the fuel is not only determined by the fuel temperature. Analyses with TESPA-ROD clearly confirm that the power density predominantly determines the strain behavior of the fuel. A strain model approach has been developed that consistently models the experimental data from the CABRI tests on UO_2 fuel. The application of this approach to experimental data of the Russian test facility BIGR (Kurchatov Institute) confirms that the strain model developed is fully valid.

FRAPCON

FRAPCON is a computer code for the transient analysis of oxide fuel rod. It was created by Pacific Northwest National Laboratory (PNL), USA.

FRAPCON-3 calculates the steady-state response of light water reactor fuel rods during long-term burnup. The code calculates the cladding temperature, internal pressure, and cladding deformation of a fuel rod as functions of time-dependent rod power and coolant boundary conditions. The phenomena modeled by the code include

- heat conduction through the fuel and cladding
- cladding elastic and plastic deformation,
- fuel-cladding mechanical interaction,
- fission gas release,
- fuel rod internal gas pressure,
- gap heat transfer between fuel cladding,
- cladding oxidation,
- heat transfer from cladding to coolant.

The code contains the necessary material properties, water properties, and heat-transfer correlations. The FRAPCON-3 code is designed to generate initial conditions for transient fuel rod analyses. Therefore, the code FRAPCON-3 provides the fuel rod initial condition for the GRS transient fuel rod code TESPA-ROD.

KENOREST

Reliable prediction of the characteristics of irradiated light water reactor fuels is needed for many aspects of the reactor operation and for the nuclear fuel cycle. Modern fuel assemblies are both heterogeneous in the distribution of fuel rods with different enrichments, in the application of gadolinium rods and in the coolant density conditions for neutron moderation.

Therefore, the 3D programme system KENOREST was developed for reactivity and full inventory calculations of LWR fuel, both with square and hexagonal assembly grids. In KENOREST, the 3D Monte Carlo code KENO and the 1D GRS burn-up programme system OREST comprising the 1D spectrum code HAMMER and 0D full inventory depletion code ORIGEN are directly coupled to the 3D reactivity and inventory calculation system. The objective is to achieve a better modelling of plutonium and actinide build-up or burnout for advanced heterogeneous fuel assembly designs. Further objectives are directed to reliable calculations of the reactivity behavior during burn-up, the pin power distributions and the reactor safety parameters for such fuel assemblies. In the most recent version of KENOREST, a multiregion model of the pellet was developed for a physically more detailed description of the radial burnout in the fuel rod. An automated convergence control for multiplication factors and pin power distributions is implemented. Updated neutronic ORIGEN libraries based on point data evaluations and additional neutronic reactions solve the Tritium, the Carbon-14 and other problems in the LWR inventory calculations.

MCNP

MCNP is a general-purpose Monte Carlo N-Particle code developed at Los Alamos National Laboratory that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport (http://mcnp-green.lanl.gov). Specific areas of application include, but are not limited to, radiation protection and dosimetry, radiation shielding, radiography, medical physics, nuclear

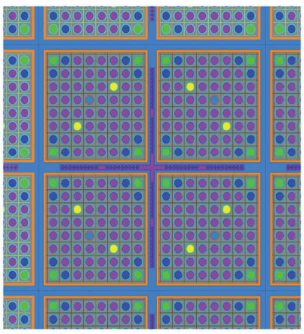
» MCNP

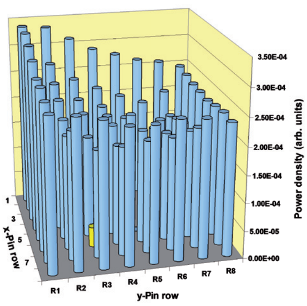
criticality safety, Detector Design and analysis, nuclear oil well logging, accelerator target design, fission and fusion reactor design, decontamination and decommissioning. There are practically no restrictions in modeling the geometry of an arrangement.

Nuclear data in continuous energy representation are typically used, although the application of group-wise data is also available. For neutrons, all reactions given in a particular cross- section evaluation (such as ENDF/B-VII) are accounted for. Binding effects in light materials like, e.g., H_2O molecules, are correctly described.

Important standard features that make MCNP very versatile and easy to use include a powerful general source, criticality source, and surface source; both geometry and output tally plotters; a variety of variance reduction techniques; a flexible tally structure; and an extensive collection of nuclear cross-section data.

At GRS, MCNP is available as a reference code for a variety of tasks within the nuclear calculation chain. It is used as a standard tool for stand-alone neutron transport calculations for critical assemblies and steady-state reactor calculations. It is also applied for high-fidelity fuel assembly depletion calculations in combination with the inventory code ORIGEN as implemented in the MONTEBURNS code; recent developments aim at coupled calculations with MCNP and a thermal-hydraulics code like ATHLET or COBRA-TF for describing stationary reactor operation states.





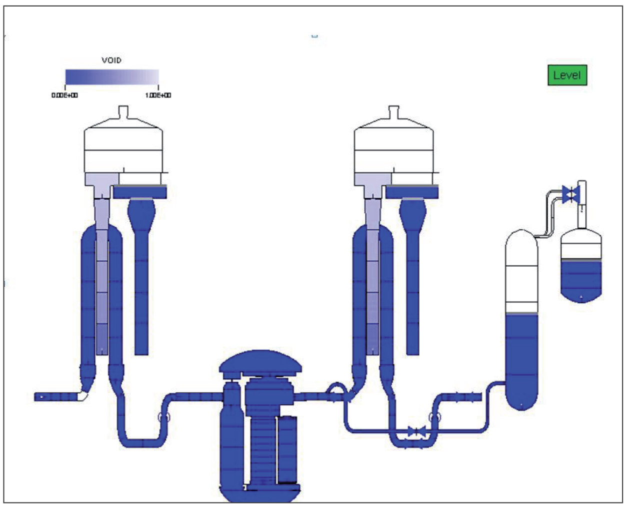
BWR Pin Power Distribution

Thermal-hydraulics and Severe Core Damage

ATHLET

The thermal-hydraulic system code ATHLET (**A**nalysis of **TH**ermal-hydraulics of **LE**aks and **T**ransients) is being developed by GRS for the analysis of the whole spectrum of leaks and transients in PWRs and BWRs. The code is applicable for western reactor designs as well as for Russian VVER and RBMK reactors. The main code features are advanced thermal-hydraulics, a modular code architecture, the separation between physical models and numerical methods, and the availability of pre- and post-processing tools.

ATHLET is composed of several basic modules for the simulation of the different phenomena involved in the operation of a light water reactor, including thermal-fluiddynamics (TFD), heat transfer and heat conduction (HECU), neutron kinetics (NEUKIN) and control and balance-of-plant (GCSM), together with the fully implicit numerical time integration method FEBE. Other independent modules (e.g. 3D neutron kinetics or containment modules) can be coupled by means of a general interface.



Automatically generated nodalization diagram for visualizing geometry and results

Thermal-hydraulics and Severe Core Damage

» ATHLET

The TFD module is based on both a five-equation system (mixture momentum equation with drift) as well as on a six-equation two-fluid model, enabling additionally the simulation of several non-condensable gases, dissolved nitrogen, and of boron transport. The system configuration to be simulated is modeled just by connecting basic thermo-fluid dynamic elements, called thermo-fluid and heat conduction objects. Multidimensional processes are simulated by parallel channels with cross flows.

The systematic validation of ATHLET is based on a well balanced set of integral and separate effects tests derived from the CSNI code validation matrices.

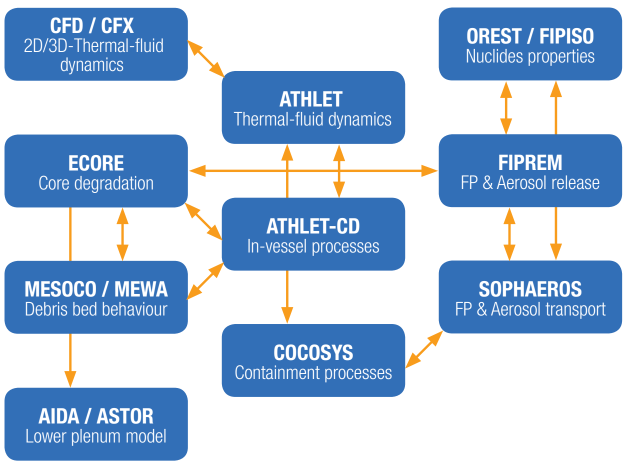
ATHLET can be applied for the simulation of operational transients, design-base and beyond design base accidents without core damage in different types of light water reactors (PWR, BWR, VVER, RBMK). Current applications are related to increase of power and enrichment, probabilistic safety analyses, core damage analyses, periodic safety analyses, boron dilution events, reactivity initiated events (3D neutron kinetics), and research reactors (e.g. FRM-2 in Garching).

ATHLET has been recently extended for the simulation of supercritical water. Moreover, different working fluids can be selected, such as heavy water, helium or lead-bismuth for the simulation of **A**ccelerator-**D**riven **S**ubcritical (ADS) systems. The program has been applied also to cryogenic hydrogen for the simulation of automotive liquid hydrogen fuel tank systems.

ATHLET-CD

The ATHLET-CD (**C**ore **D**egradation) code has been developed and validated for accidents resulting in major core damage. The development and integration of models in ATHLET-CD is done in close co-operation with the Institut für Kernenergetik und Energiesysteme (IKE), of the University of Stuttgart. By the models for the formation and movement of metallic and ceramic melts in the core area and the thermal behavior of particle beds, as well as for the release of fission products and aerosols in the core area and their transport and deposition in the cooling circuit, the application range of the computer code has been extended significantly.

This is demonstrated by successful post calculations of bundle and integral experiments, such as CORA, QUENCH, LOFT-LP-FP2 and Phebus FP, or the TMI-2 accident and the incident at Paks-2 (NEA 2008). As demonstrated by the calculation performed for Phébus FPT1 within the framework of the International Standard Problem (ISP-46), full plant simulations can be performed with the version coupled with COCOSYS. The ATHLET-CD structure is modular, both to provide a variety of models for the simulation and to provide an optimum basis for further development. For a comprehensive simulation of the thermal-fluid dynamics in the nuclear steam supply system, the ATHLET system code has fully been integrated.



The components of ATHLET-CD core system

» ATHLET-CD

The ECORE module consists of models for fuel rods, control rods (Ag, In, Cd and B4C) and fuel channels. The module describes the mechanical fuel rod behavior (ballooning), the oxidation of zirconium and boron carbide, dissolution of fuel by zirconium and of boron carbide by steel, as well as melting of metallic and ceramic components. The model takes into account oxidation, freezing, re-melting, re-freezing and the formation and dissolution of blockages. Steam consumption and hydrogen generation by oxidation and the flow blockage are taken into account in the fluid dynamics model.

Besides the convective heat transfer, modelling also covers the heat radiation between the fuel rods and the surrounding core structures. The FIPREM module describes the release of fission products and aerosols.

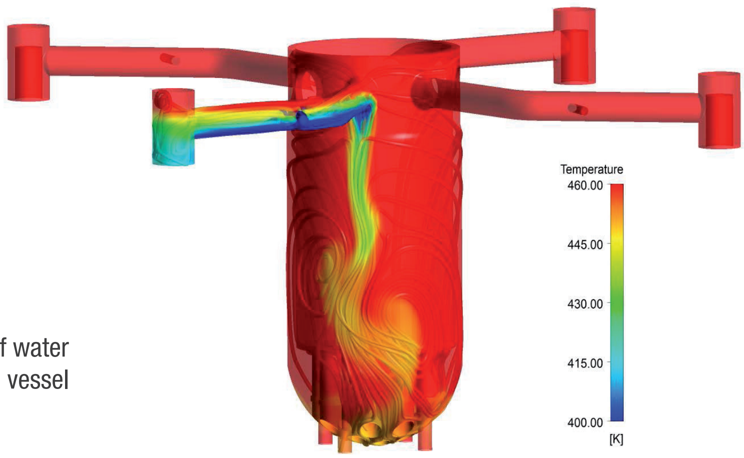
Transport and retention of aerosols and fission products in the coolant system are simulated by the SOPHAEROS code, developed by the Institut de Radioprotection et de Sûreté Nucléaire (IRSN).

The module MEWA for simulation of the debris bed has already been implemented in ATHLET-CD. It has its own fluid dynamics for the flow in porous media and is coupled to the ATHLET fluid dynamics on the outer boundaries. The transition of the nearly intact core geometry (ECORE) to debris bed (MEWA) depends on the local degree of core degradation.

CFX

ANSYS CFX (http://www.ansys.com) is a commercial multiphase Computational Fluid Dynamics (CFD) code, which is capable to predict three-dimensional fluid flow behavior in complex geometries and can provide detailed distributions of the physical parameters in space and time. It is widely used in the oil, automotive, power generation, marine, aviation and other industries. ANSYS CFX is a general purpose CFD software program that combines an advanced solver with powerful pre- and post-processing capabilities. It is an efficient tool for simulating the behavior of systems involving fluid flow, heat transfer, chemical, combustion and other related physical processes. The 3D CFD code uses a unique hybrid finite-element/finite-volume approach to solve the Navier-Stokes equations. Moreover, various turbulence models have been integrated in the program to allow realistic simulation of physical processes in wide range of industrial and academic applications.

Within the frame of a concerted activity for "Development and Application of CFD Programmes for Phenomena in the Primary System of Light Water Reactor" under the lead of GRS, a CFD-software package for the efficient and accurate simulation of reactor safety relevant fluid flow and heat transfer processes is being developed.



Injection of water
into the reactor pressure vessel

» CFX

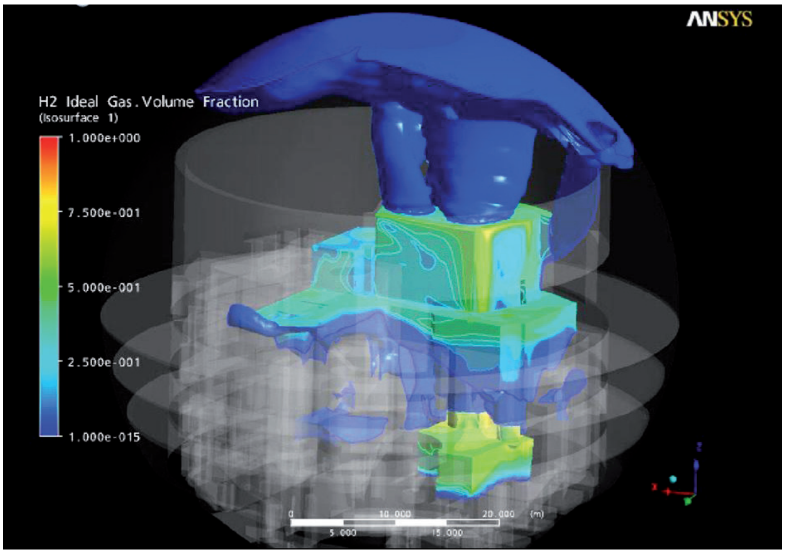
The investigations are primarily concerned with three-dimensional flows in the primary system of pressurized water reactors, and containments.

In the field of fluid dynamics, GRS is involved in the development of the coupled code ATHLET-CFX. With such advanced simulation strategy, parts of the primary circuit with relevant 3D effects such as simulation of 3D flows with high spatial resolution and coolant mixing processes are treated with CFX, and ATHLET is used to provide fast solution for the flow behavior in those areas where 1D simulation is adequate.

CFX is also used for the simulation of gas distribution in a reactor containment in the case of a severe accident. Activities for the code validation and application in this topic are sponsored by the BMWi. Actual research topics are additional models for condensation processes or recombiners, turbulence modelling, H_2 deflagration and combustion models. A geometrical model for the containment has been developed for the simulation of severe accident scenarios, as in the figure below.

Verification and validation activities for the CFD code ANSYS CFX are being performed at GRS within numerous national and international projects, e.g. ECORA, NURESIM, NURISP, THINS. These are not based only on small academic experiments, but also on large scale experimental data from UPTF, LSTF and ROCOM facilities. Moreover, GRS participates in international validation initiatives like the Vattenfall T-Junction, PSBT and BFBT benchmarks. In a next step, ANSYS CFX will be further developed for the simulation of liquid metal cooling media used in some Generation IV reactor concepts.

The models which are used for the gas distribution and condensation processes were validated by comparison to results of ThAI-, PANDA- and Battelle-Modell-Containment experiments. H_2 deflagration and combustion models were validated by comparison to experiments of the RUT-facility, the Battelle-Modell-Containment and to ENACCEF experiments.

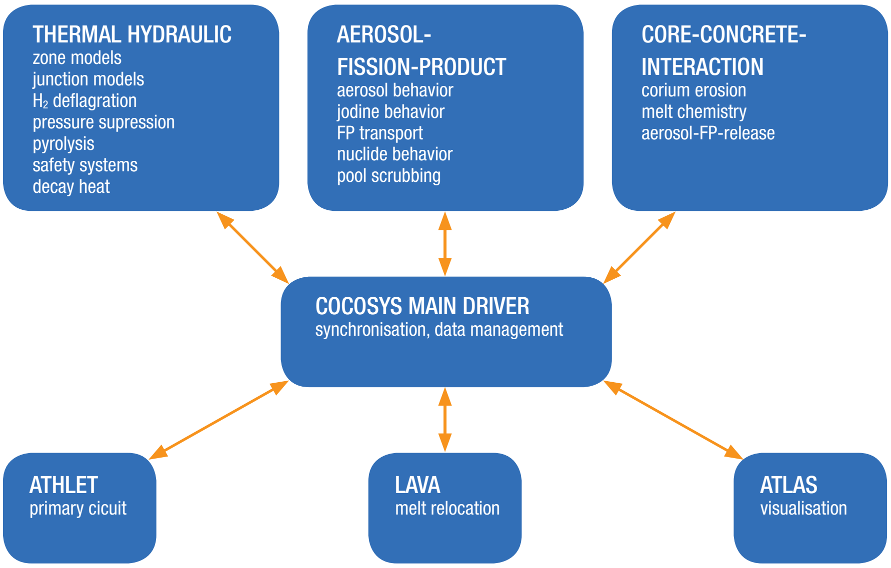


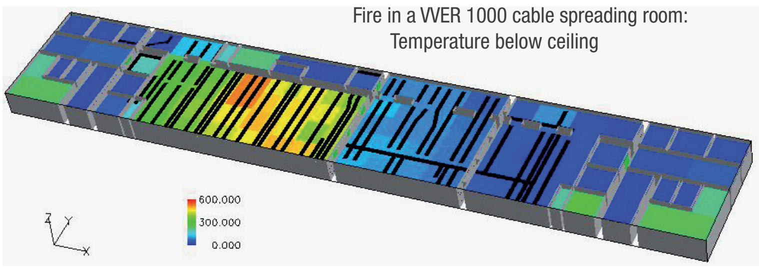
Hydrogen concentration
in the containment

COCOSYS

The simulation of design basis and severe accident propagation in containments of nuclear power plants is required for the analysis of the potential consequences of severe accidents and possible counter measures under conditions as realistic as possible. Therefore, at GRS the **CO**ntainment **CO**de **SYS**tem (COCOSYS) has been developed. The main objective is to provide a code system on the basis of mechanistic models for the comprehensive simulation of all relevant phenomena processes and plant states during severe accidents in the containment of light water reactors, also covering the design basis accidents.

In COCOSYS mechanistic models are used as far as possible for analysing the physical-chemical processes in containments. Essential interactions between the individual processes, like e.g. between thermal hydraulics, hydrogen combustion as well as fission product and aerosol behavior will be treated in an extensive way. With such a detailed approach, COCOSYS is not restricted to relevant individual severe accident phenomena, but will also make it possible to demonstrate the interactions between these phenomena as well as the overall behavior of the containment.





Visualization of COCOSYS simulation results

» COCOSYS

The complete system is divided into several so-called main modules. Each main module is a separately executable program, dedicated to one specific area of the overall problem. Communication among these main modules is effected via PVM, which organises and controls the calculation sequence. The individual main modules calculate the overall problem in such a way that they can be coupled at time-step level, which means that the extent of the parameters that have to be exchanged is relatively low. To keep the complexity of the data exchange within reasonable limits, any data exchange is only allowed between the main modules and the COCOSYS driver.

The **T**hermal **HY**draulic (THY) main module is a so-called lumped-parameter model. The compartments of the considered power plant, test facility or other building types have to be subdivided into control volumes (zones). The thermal-dynamic state of a zone is defined by its temperature(s) and masses of the specified components. Beside the usual equilibrium and non-equilibrium zone model, specific zone models (DRASYS and VORTEX) to simulate pressure suppression systems have been implemented. The junction models describe the flow interaction between different zones. In COCOSYS, the simulation of gas flow and water drainage is strongly separated, although water can be transported via atmospheric junctions by gas flow and dissolved gases can be transported via drain junctions. For an adequate simulation of the different systems or boundary conditions, specific junction models are implemented, like rupture discs, atmospheric valves, flaps/doors and specific pressure relief valves used in Russian types reactors. The walls, floors and ceilings of the considered building are represented by structure objects. The structure objects include all types of metallic and non metallic heat sinks within zones and between them. For the simulation of severe accident sequences and possible accident management measures it is necessary to take safety systems into account. The main thermal-hydraulics module was extended to include the simulation of oil and cable fires. In the case of the oil fire, the burnt material is simulated by a structure with fixed temperature grid.

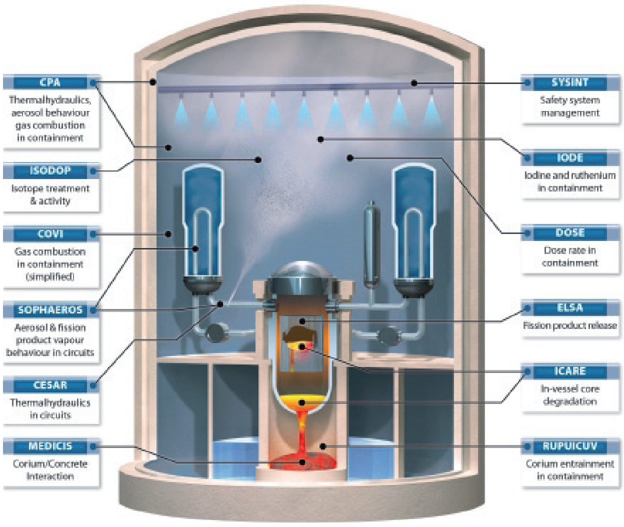
The **A**erosol-**F**ission-**P**roduct (AFP) main module is used for best-estimate simulations of the fission product behavior in the containment of LWRs. Both the thermal hydraulic (THY) and the aerosol-fission-product (AFP) main modules consider the interactions between the thermal hydraulics and aerosol fission product behavior. The following deposition processes are covered: sedimentation, diffusive deposition, thermophoresis and diffusiophoresis. The FIPHOST module calculates the transport of the fission products within the containment. The fission products are treated as the radioactive part of the aerosol particles and the radioactive non-condensable gases, whereas their mass is not considered in the model. Nuclide behavior is simulated with the help of the FIPISO module. FIPISO considers the reactor's initial core inventory (pre-calculated by other codes) and calculates on this basis the decay of the fission products according to the time of the onset of the release by using established nuclide libraries (analogous to ORIGIN). The chemistry in the AIM-3 iodine module contains approximately 70 different reactions. AIM-3 distinguishes between 16 iodine species in the atmosphere and 10 iodine species in the sump. It calculates iodine transport between atmosphere and sump as well as across the compartments. The retention of aerosols during gas transport through water pools is calculated by the SPARC-B module. This allows among other things the simulation of "pool scrubbing" in the pressure suppression system of a boiling water reactor.

The data can be visualised both online and offline with the ATLAS program.

ASTEC

Since several years, the French Institut de Radioprotection et de Sûreté Nucléaire (IRSN) and the German Gesellschaft für Anlagen und Reaktorsicherheit mbH (GRS) have been jointly developing “integral” code ASTEC (**A**ccident **S**ource **T**erm **E**valuation **C**ode) to simulate the complete scenario of a hypothetical severe accident in a nuclear water-cooled reactor, from the initial event until the possible radiological release of fission products out of the containment into the environment. ASTEC is in particular extensively used by European partners in the frame of the SARNET excellence network of the European Commission’s 6th and 7th FP.

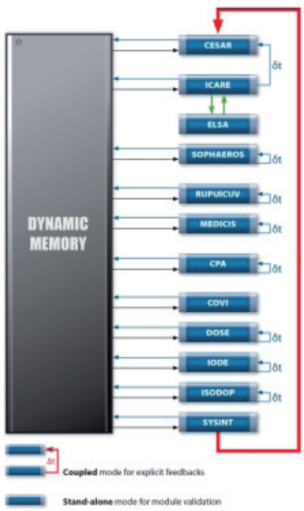
The code structure is modular, each of its modules simulating a reactor zone or a set of physical phenomena. The modules of ASTEC are shown in the figure below. Data are exchanged between the ASTEC modules at macro time steps through a dynamic database, i.e., evolving throughout the calculation and mirroring at each time the state of the reactor. The explicit coupling at each numerical macro time step allows making easier the validation of a given module or a subset of modules. A specific tool, SIGAL-ODESSA, was developed for managing this database. The programming language is Fortran 95. The code size is about 350 000 lines, distributed in more than 1000 routines. The code runs on a PC in diverse environments such as Linux or Windows, or on UNIX workstations.



The current version allows complete calculations of different severe accident sequences on French, German and Russian type PWRs operating at full power, such as station black-out, loss of steam generator feed-water, steam generator tube rupture, as well as small, medium and large break loss of coolant accidents.

The code validation benefits greatly from the very intensive work performed over more than 15 years with the precursor codes (ESCADRE, RALOC, and FIPLOC) and with the ICARE2 code. Many ISP OECD exercises were selected for validation: BETHSY, PACTEL, CORA-13, VANAM M3, THAI, etc., as well as the ISP46 Phébus FPT1 calculation as examples of integral calculations coupling most modules. In addition, most code modules are used for the detailed interpretation of all the integral Phébus FP experiments, e.g., SOPHAEROS for FP behavior in the circuit. All this IRSN-GRS work was completed by validation done by the SARNET partners. On the whole, the status of validation can be judged satisfactory; it shows that the code reflects the state of the art in terms of understanding and modeling in particular with view to FP behavior. Like all other integral codes, the main necessary V2 model improvements concern MCCI, reflooding of degraded cores, and extension to BWR.

ASTEC is further deployed to PSA level 2 analyses (including uncertainty analyses), for studying accident management, preventive or mitigative measures in accidents, for analyzing scenarios in order to increase the phenomenological understanding, and to accompany experiments. Long term perspectives include also the extension of ASTEC to GEN IV type Sodium Fast Reactors (SFR).



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Modules in ASTEC

Thermal-hydraulics and Severe Core Damage

MELCOR

Since 1993, GRS uses the code MELCOR for deterministic analyses of beyond design-base accidents resp. severe accidents with core damage in PWR- and BWR power plants. The analyses are made to support the development of accident management measures and as a basis for PSA level 2 analyses.

MELCOR is an integral code being developed at Sandia National Laboratories on behalf of the US Nuclear Reactor Commission, and is available to all member states within the Cooperative Severe Accident Research Program at no charge.

The following short description is extracted from the MELCOR web page at http://melcor.sandia.gov:

MELCOR is a fully integrated, engineering-level computer code whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. A broad spectrum of severe accident phenomena in both boiling and pressurized water reactors is treated in MELCOR in a unified framework. Current uses of MELCOR include estimation of fission product source terms and their sensitivities and uncertainties in a variety of applications.

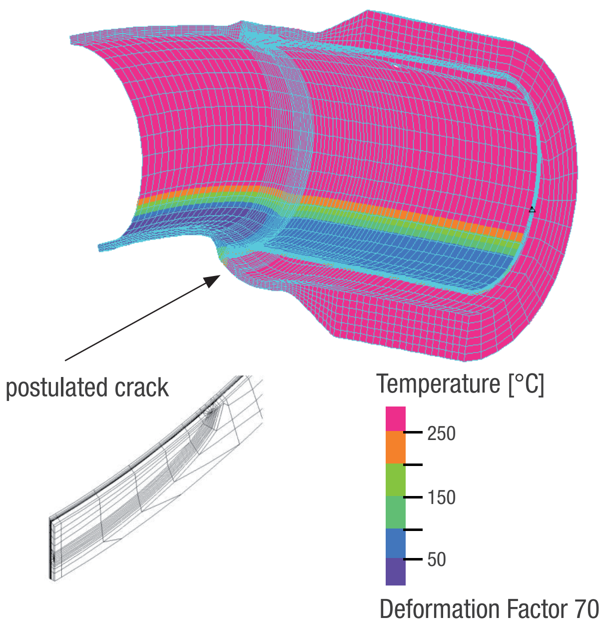
The MELCOR code is composed of an executive driver and a number of major modules, or packages, that together model the major systems of a reactor plant and their generally coupled interactions. Reactor plant systems and their response to off-normal or accident conditions include:

- Thermal-hydraulic response of the primary reactor coolant system, the reactor cavity, the containment, and the confinement buildings
- Core uncovering (loss of coolant), fuel heatup, cladding oxidation, fuel degradation (loss of rod geometry), and core material melting and relocation
- Heatup of reactor vessel lower head from relocated fuel materials and the thermal and mechanical loading and failure of the vessel lower head, and transfer of core materials to the reactor vessel cavity
- Core-concrete attack and ensuing aerosol generation
- In-vessel and ex-vessel hydrogen production, transport, and combustion
- Fission product release (aerosol and vapor), transport, and deposition
- Behavior of radioactive aerosols in the reactor containment building, including scrubbing in water pools, and aerosol mechanics in the containment atmosphere such as particle agglomeration and gravitational settling
- Impact of engineered safety features on thermal-hydraulic and radionuclide behavior
- The various code packages have been written using a carefully designed modular structure with well-defined interfaces between them. This allows the exchange of complete and consistent information among them so that all phenomena are explicitly coupled at every step. The structure also facilitates maintenance and upgrading of the code.

Structural Mechanics

ADINA

Within the frame of safety-related structural mechanical issues the universal Finite-Element-program system ADINA (**A**utomatic **D**ynamic **I**ncremental **N**onlinear **A**nalysis) is applied. GRS uses the code for development and validation of structural mechanics analysis methods for integrity assessment of nuclear components under accident loading like reinforced concrete containment structures. Areas of application are e.g. the load-bearing capacity of reinforced concrete structures with and without pre-stressing, integrity assessment of vessels and piping under mechanical and thermal transient loads including fracture mechanical aspects concerning behavior of postulated cracks, the behavior of the reactor pressure vessel and piping during core melt scenarios, accident management measures, water hammer and earthquakes, as well as the behavior of fuel element cladding tubes during loads resulting from loss-of-coolant accidents. An overview of the capabilities of the program system ADINA is shown on http://www.adina.com/ including a collection of analyses examples for structural mechanical issues.



Temperature distribution
in feed water nozzle
with postulated crack

Loading:
thermal stratification
ΔT = 250°C, p = 6,6 MPa

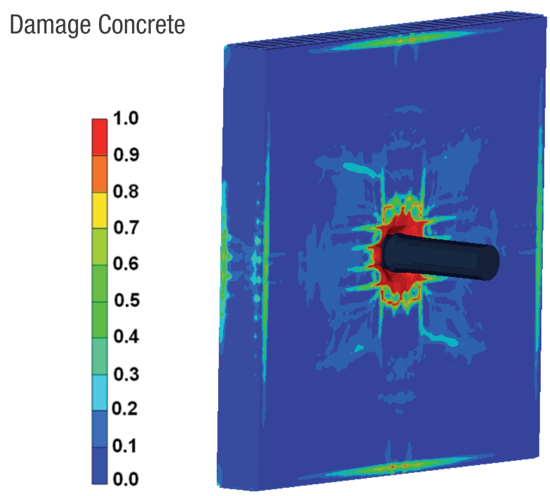
PROST

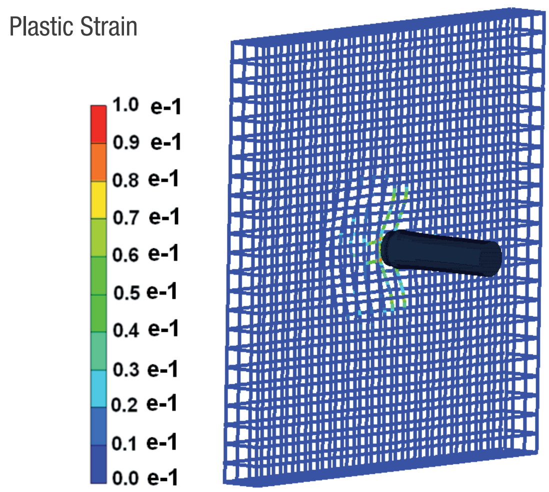
GRS develops a probabilistic analysis tool PROST (**PRO**babilistic **ST**ructure calculation) for the determination of structural reliability of piping and vessels. This program development allows the calculation of leak- and break probabilities for various geometries, load assumptions, material properties and crack assumptions with consideration of uncertainties in form of distribution functions. With the developed prototype the leak- and break probabilities can be determined as function of the operating time taking into account the damage mechanism "fatigue" on the basis of a two-parametric fracture mechanics failure criterion. Furthermore, a module was developed taking into consideration the damage mechanism "corrosion", especially inter-granular stress crack corrosion with austenitic materials and strain-induced crack corrosion with ferritic materials. Additionally, an available method for leak rates calculations have been included into the program, because leak detection has a noteworthy influence on the break probability, since measures can be taken into consideration due to indications of leak monitoring systems installed in nuclear power stations. The application range of the code was extended to complex geometries in regards to loading and boundary conditions by additional code modules to include the results of finite element (FE) calculations.

Structural Mechanics

AUTODYN

The commercial software ANSYS AUTODYN is an analysis code for structural dynamics with explicit time integration. It is developed in particular to simulate the dynamic and nonlinear behavior of materials undergoing large deformations at high strain rates. ANSYS AUTODYN is used in defence industry but also in several other branches of industry as well as in different fields of research and education. Typical applications are for instance the simulation of impact and penetration events, propagation of shock waves, explosions, material forming and crashworthiness. Ductile, brittle and composite solid materials, liquids and gases including high explosives can be modelled, whereby interaction of different bodies in different aggregate states can be considered. For this several current numerical processors (Finite Elements, Euler approaches, Smoothed Particle Hydrodynamics, Arbitrary Lagrange-Euler) are available and may be coupled among each other. Furthermore, ANSYS AUTODYN is more and more integrated in the ANSYS WORKBENCH. This enables the straightforward coupling with other ANSYS products especially for pre- and post-processing. GRS uses ANSYS AUTODYN for the simulation of impacts of potential missiles like aircraft structures on reinforced concrete structures, which have to be assessed with respect to their load carrying capacity. In this context the code capabilities are investigated by simulations of selected impact tests of different scales carried out at different facilities.





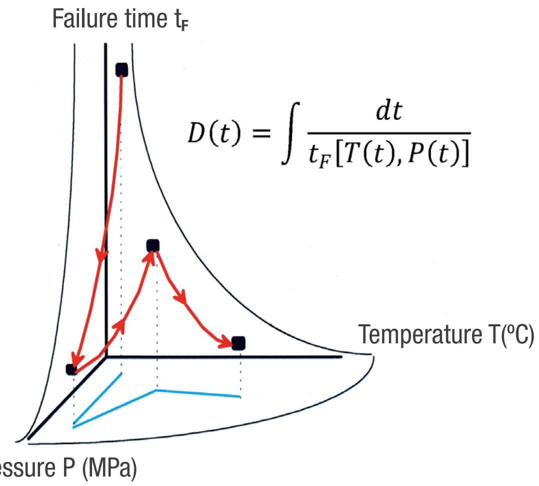
AUTODYN
Simulation of a large scale impact test

WINLECK

For the estimation of discharge flow rates through crack-like leaks in pipes for subcooled water up to saturated steam conditions analytical one-dimensional models based on the definition of a thermal-hydraulic diameter were provided. Applications with these leak rate models indicate that partly these models lead to unsatisfactory results. Therefore, from the results of about 180 leak rate tests performed by various institutions in different countries an empirical model was developed in form of a four-factor-formula, providing an overall better approximation of the available tests than the other one-dimensional models. The addressed leak rate models are made available in the WINLECK program developed by GRS.

ASTOR

The ASTOR program (**A**pproximated **S**tructural **T**ime **o**f **R**upture) has been developed as a simplified procedure for the integrity assessment of RPVs and piping loaded under internal pressure and high temperatures concerning failure times. With time-varying loads the appropriate load path in the pressure-temperature-area is pursued for the determination of the failure time. Using a linear damage accumulation hypothesis the arising damage increments per time unit is added up. When this summation reaches the damage value 1 during the transient then this point of time is termed as failure time of the component. A damage increment on the load path in the pressure-temperature-area is determined by the inverse of the failure time (for the pressure-temperature level of the considered time increment) taken from a damage surface based on Finite Element (FE-) analyses for selected pressure and temperature levels. In addition ASTOR for RPV was extended to transient temperature loads with hotspot, whereby the temperature maximum within the hotspot area and a variable hotspot width has been introduced as additional parameters. During further development of the simplified method it should be observed, that the number of parameters characterizing the geometry, the material properties and the loads to be covered is kept as low as possible in order to limit the amount of FE-analyses to be conducted for the damage surface.



Linear Damage Accumulation Hypothesis in ASTOR

Tools applicable with several codes

Uncertainty, Sensitivity and Probabilistic Dynamic Analysis

SUSA

Along with the development and application of computer codes, it has been increasingly recognized that the corresponding computational results are associated with uncertainty due to lack of knowledge on various sources. Therefore, uncertainty and sensitivity analyses are performed to get (1) a quantification of the combined influence of many of these uncertainty sources and (2) a ranking of the individual sources according to their contribution to the uncertainty of the results.

The software tool SUSA (**S**oftware for **U**ncertainty and **S**ensitivity **A**nalyses) guides through the main steps of a probabilistic uncertainty and sensitivity analysis. These steps can be summarized as follows:

1. Identification of all phenomena, modeling assumptions, and parameters that are potentially important contributors to the uncertainty of the computational result and representation of all uncertainty sources by uncertain parameters.

2. Quantification of the state of knowledge on the uncertain parameters in terms of probability distributions and dependence measures.

3. Generation of a sample of values for the uncertain parameters according to a multivariate probability distribution which satisfies the input given in step 2.

4. Performance of computer code runs for each set of values sampled for the uncertain parameters -> random sample from the unknown probability distribution of the computational result.

5. Quantification of the uncertainty of the computational result on the basis of the sample resulting from step 4.

6. Ranking of the parameters with respect to their contribution to the overall uncertainty of the computational result (Sensitivity Analysis).

7. Comprehensive documentation of the analysis steps for scrutinizing the analysis results.

SUSA combines well established concepts and tools from probability calculus and statistics with a comfortable menu-driven user interface. All data transfers, statistical data analyses and graphical representations are performed automatically. SUSA even provides a comprehensive documentation of the analysis steps for scrutinizing the analysis output.

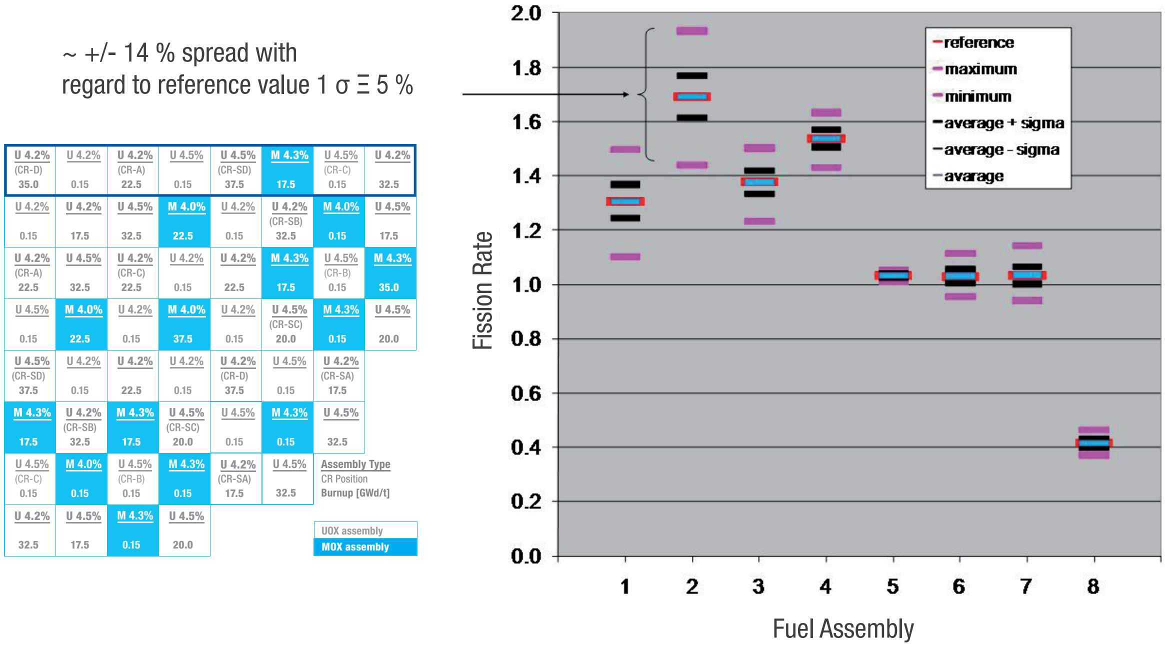
Various types of probability distributions and dependence structures are available for modeling uncertainty probabilistically. For sample generation, the simple random sampling or the Latin Hypercube sampling procedure may be applied. In principal, the runs of any computer code can be started from within SUSA. SUSA can even provide input decks of complex computer codes each accounting for a different set of parameter values. Diverse alternatives exist for quantifying the uncertainty of the computational results (e.g. tolerance limits) and their sensitivity with respect to the individual uncertainty sources (e.g. correlations, regression based measures or correlation ratios).

SUSA is a PC-software running under Windows (NT, XP or Windows 7). The current version 3.6 requires the installation of MS Excel 2003, 2007, or 2010. It can be used for any simple or complex application. There are, in principal, no limitations concerning the number of uncertain parameters, output quantities, and computer code runs.

XSUSA

The sampling based GRS uncertainty and sensitivity software XSUSA (Cross **S**ection **U**ncertainty and **S**ensitivity **A**nalysis) has been developed for the use with nuclear data uncertainties as contained in the nuclear covariance matrices. To this end, many calculations for the problem under consideration are performed with varied input data. The variations of the input data are generated randomly from the given probability distributions of the parameters including possible correlations between them. When dealing with nuclear data and their uncertainties as contained in the covariance matrices, only the first two moments of the distributions (expectation values and covariances) are known. Due to this lack of information, the distributions are assumed to be of Gaussian shape. After performing all the calculations (typically 100 or more), the output quantities of interest are statistically analyzed, and their uncertainty ranges and sensitivities to the input parameters are determined.

As code system for the nuclear calculations, the SCALE-6 system is chosen. It has the advantages that it contains comprehensive sets of up-to-date nuclear cross sections as well as covariance data and almost all codes needed for the desired calculations, codes and data are well matched, and both data and source code are open. The tools necessary for varying the nuclear data corresponding to the sampling results, as well as handling the nuclear data in all steps of the calculation chain, have been developed within the XSUSA system. As transport solvers, the 1D S_N code XSDRN so far has been used for pin cell criticality calculations, the 2D general geometry S_N code NEWT for spectral calculations, including few-group cross section generation, and the 3D Monte Carlo code KENO for stationary reactor core calculations. The propagation of uncertainties through depletion calculations with TRITON/NEWT is in preparation and has already been tested on a fuel assembly depletion calculation. All these transport codes are part of the SCALE-6 system. In certain cases, also the 3D Monte Carlo code MCNP in multi-group mode has been applied.



MCDET

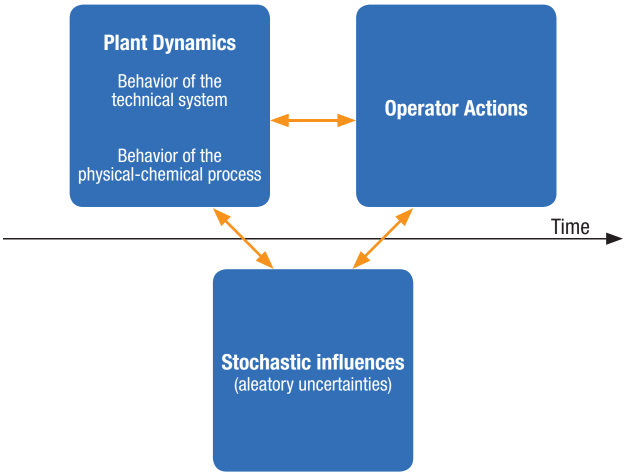
The accident scenarios to be considered in a PSA are characterized by complex interactions over time between the plant behavior, operator actions and stochastic influences.

Due to stochastic influences or more specifically due to aleatory uncertainties on
- the behavior of the technical system,
- the performance of the plant operators,
- the behavior of the physical-chemical process and
- on external factors

a variety of potential event sequences has to be considered, and the assessment of the consequences of an accident scenario can only be probabilistic. It is obvious, that the spectrum of event sequences may be tremendous, if aleatory uncertainties exist, for instance, on the physical-chemical process or on the timing of system function failures and of human actions. Only if a PSA is able to account for all the sequences which may evolve and to rank the sequences according to their likelihood, it can provide a well-founded probabilistic assessment. But the conventional PSA approach may not be capable of doing that, because

- it is not an integral analysis where the interaction between the plant behavior, operator actions, and stochastic influences can be captured,
- it has no time axis and, therefore, cannot adequately account for the influence of the timing,
- it is decoupled from the physical-chemical process and therefore cannot adequately account for the influence of variations in the process, and
- it strongly depends on the experts who build the models (expert-to-expert variation).

The MCDET method allows for an integral probabilistic analysis of accident scenarios. The combination of Monte Carlo (MC) simulation and the Discrete Dynamic Event Tree (DDET) approach is capable of accounting for any aleatory uncertainty at any time. The implemented MCDET modules can in principal be coupled with any deterministic dynamics code simulating the behavior of a nuclear power plant under accident conditions (like, for instance, ATHLET, RELAP or MELCOR). Beside aleatory uncertainties, MCDET can also consider epistemic uncertainties which determine how precise probabilistic assessments can only be provided due to the knowledge uncertainties involved in the calculation.



The MCDET modules were supplemented by a crew module which enables calculating the dynamics of crew actions depending and acting on the plant dynamics as modeled in a deterministic code and on stochastic influences as considered in the MCDET modules. The crew module allows for running situation-dependent sequences of human actions as they are expected for a dominant cognitive behavior.

The capacity of the MCDET modules and the crew module has been demonstrated by several applications including a large-scale station black-out scenario and the analysis of an emergency operating procedure.

Simulation environment

ATLAS

Today, complex computer codes allow the simulation of many different processes in nuclear power plants, from normal operation up to severe accidents. The operation of these codes and the evaluation of the results is, however, difficult and requires a high level of expert know-how. The possibilities of present-day computer technology make it possible to simplify the use of simulation codes by way of modern user interfaces and graphic processing of results.

One important tool in this area is the ATLAS analysis simulator developed by GRS. It allows the representation and assessment of the computation results with the help of modern visualization methods. It also provides the possibility of interactive control of the simulation, with intervention possibilities similar to those of a real power plant.

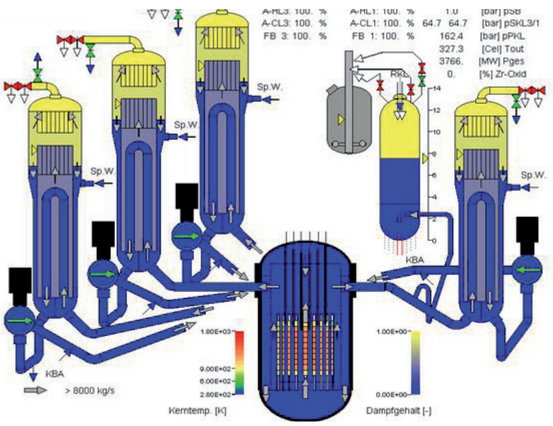
The underlying objective of the development of ATLAS was to provide an integrative simulation environment for different models where the resulting data can be graphically represented and the simulation sequence interactively controlled. Currently there are a number of dynamic simulation codes available in ATLAS, covering a wide spectrum of reactor safety analyses. They presently include

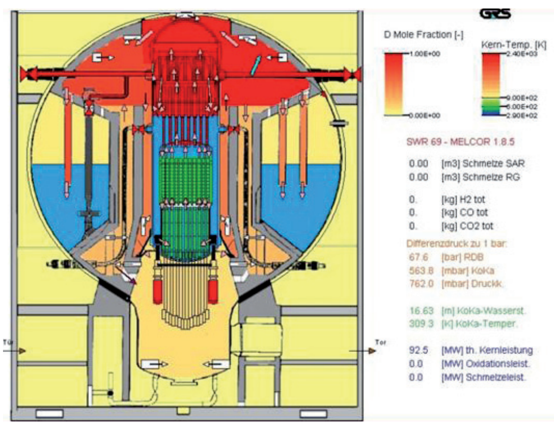
- ATHLET/ ATHLET-CD (GRS, reactor coolant system and ancillary systems)
- COCOSYS (GRS, reactor containment and containment structure)
- ASTEC (GRS and IRSN, overall plant)
- MELCOR (SNL, overall plant)
- S-RELAP (AREVA, reactor coolant system and ancillary systems)

These codes comprise models for the reactor coolant system with thermal hydraulics and heat transfer, for reactor systems and instrumentation & control, for neutron dynamics, for core degradation processes and for the pressure build-up and fission product behavior in the containment.

ATLAS can be used on different computer systems. At its analysis center at Garching near Munich, GRS provides a special infrastructure for the application of ATLAS which is similar to a power plant digital control room.

ATLAS is currently used by research and regulatory organizations worldwide for a wide range of tasks. Particularly noteworthy are the detailed analysis simulators developed on behalf of the Federal Environment Ministry for the German nuclear power plants, the performance of so-called Human Factor analyses, the training of personnel in the area of severe accidents, and the application as a visualization tool for various computer codes.





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