

F. Weyermann, C. Spengler, P. Schöffel, S. Buchholz, T. Steinhoff, M. Sonnenkalb, A. Wielenberg and A. Schaffrath

# Development of AC<sup>2</sup> for the simulation of advanced reactor design of Generation 3/3+ and light water cooled SMRs

The transition from Generation 2 to Generation 3/3+ and 4 reactors, as well as the development of small modular reactors (SMR), place new demands on computational programs designed to simulate conditions of normal operation, operational occurrences, design basis accidents and severe accidents. On the one hand, most passive safety systems of advanced and innovative plants operate at low pressures even down to vacuum conditions and the driving forces are low compared to active systems. On the other hand, the containment is no longer just a barrier to retain radioactive material in the event of leakage of the cooling system, but it is an important link in the passive cooling chain. This requires an expansion and improvement of the existing simulation programs for the cooling circuit and containment, as well as the realization of a coupling between these simulation programs. The new AC<sup>2</sup> program package combines the proven simulation codes ATHLET/ATHLET-CD and COCOSYS in one software suite to hit this target. The individual components of the suite are continuously extended and validated for their application to novel safety systems. This makes it possible to simulate the entire spectrum of accidents for Generation 3/3+, 4 and light water cooled SMR systems with just one program package. This publication gives an overview of the current state of development of AC<sup>2</sup> and its individual modules.

**Aktuelle Entwicklungen des Programms AC<sup>2</sup> zur Berechnung von fortschrittlichen Reaktorkonzepten der Generation 3/3+ sowie von leichtwassergekühlten SMR-Konzepten.** Der Übergang von Reaktoren der Generation 2 nach Generation 3/3+ und 4 und auch das Aufkommen von kleinen modularen Reaktoren (engl. Small Modular Reactors = SMR) stellt an Rechenprogramme zur Simulation von Betriebszuständen, Transienten, Stör- und Unfällen in Kernkraftwerken neue Anforderungen. Zum einen arbeiten die in fortschrittlichen und innovativen Reaktoren eingesetzten passiven Sicherheitssysteme teilweise bei sehr niedrigen Drücken bis hinab zu Vakuumbedingungen und auch die treibenden Kräfte sind im Vergleich zu aktiven Systemen gering. Zum anderen ist der Sicherheitsbehälter (Containment) nicht mehr nur eine Barriere zum Aktivitätseinschluss im Falle von Leckagen des Kühlsystems, sondern es ist ein wichtiges Glied der passiven Wärmeabfuhr. Das erfordert zum einen eine Erweiterung und Verbesserung der bestehenden Simulationsprogramme für Kühlkreislauf und Containment, aber auch die Realisierung einer Kopplung zwischen diesen beiden Simulationsprogrammen. Unter dem Namen AC<sup>2</sup> wurden zu diesem Zweck die erprobten Simulationsprogramme ATHLET/ATHLET-CD und COCOSYS in einem

Programmsystem vereint. Dieses wird kontinuierlich für die Anwendung auf neuartige Sicherheitssysteme und Anwendungsbereiche erweitert und validiert. Somit ist es möglich mit nur einem Programmsystem das gesamte Störfallspektrum für Anlagen der Generation 3/3+, 4 und leichtwassergekühlter SMRs zu simulieren. Dieser Aufsatz gibt einen Überblick über den aktuellen Stand der Entwicklung von AC<sup>2</sup> und seiner Einzelmodule.

## 1 Introduction

Reactor designs of generation 3 and 3+ feature several evolutionary, state-of-the-art design improvements compared to generation 2 plants, which account for most plants currently in operation worldwide [1]. These improvements are in the areas of fuel technology, thermal efficiency, modularized construction, standardized design and safety systems, especially the use of passive rather than active systems. In these Generation 3/3+ plants like the AP1000, CAP1400, HPR-1000, WWER-1200 or advanced boiling water reactors like the ABWR, the (E)SBWR or the KERENA (concept) the containment is an important part of the emergency cooling chain. In case of a loss of coolant accident (LOCA), the heat released to the containment via the leak and the passive core cooling systems (e.g. emergency condensers, automatic depressurization systems, see KERENA, AP1000, CAP1400...) is removed by specific design features and finally transferred to the environment as the ultimate heat sink. Also, small modular reactors (SMRs), which are currently under development (e.g. NuScale, Carem, CAP200, KLT-40S, SMART, I-150) show such a close connection between the cooling circuit and the containment.

This interconnection of the cooling circuit and the containment using passive safety features with small driving forces does not allow for an effective decoupling of simulation domains and thus puts new and challenging demands on simulation programs used in safety demonstration. In the past for the thermal hydraulics simulation of generation 2 plants, the containment was generally represented by a suitably conservative simplified model. For the simulation of the cooling circuit, system codes like ATHLET, RELAP or CATHARE have been used with the containment being simulated as a simple pressure and temperature boundary condition or using a very rough representation of the containment. For the simulation of the pressurization and temperature rise under LOCA conditions or main steam line breaks in the contain-

ment lumped parameter codes like COCOSYS, CONTAIN, WAVCO or GOTHIC have been used with a precalculated leak mass flow rate from the cooling system into the containment. Further, such containment codes have been necessary to predict fission product and aerosol behaviour in the containment with view to any source term to the environment as consequence during severe accidents. For realistically simulating the behaviour of passive safety features of Generation 3/3+ plants and SMRs, which closely interact with the specific containment behaviour, best-estimate simulations for both containment and cooling circuit simulation domains are the state of the art. This is possible in principle by using integral codes such as ASTEC, MAAP or MELCOR. However, as these integral codes generally come with limitations in details of modelling and treatment of phenomena, using closely coupled best-estimate codes for the circuit and the containment is a further promising alternative. This is one rationale for on-going integration of the GRS codes ATHLET, ATHLET-CD and COCOSYS into the program suite AC<sup>2</sup>.

In the following the three main programs of AC<sup>2</sup> are described in detail and the coupling abilities of the modules are presented. Also, an overview on the quality assurance of the code development is given.

## 2 Description of AC<sup>2</sup> components

AC<sup>2</sup> is a coupled code system developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH for the simulation of normal operation, anticipated operational occurrences, design and beyond design basis up to severe accidents in LWR and basic capabilities of other reactor designs. It consists of three main modules (see also Fig. 1):

- ATHLET, which is used for the detailed thermohydraulic simulation of normal operation, transients and loss of coolant accidents up to design extension conditions without core degradation of the reactor coolant system,
- ATHLET-CD, which is the extension of ATHLET for the simulation of design extension conditions with core degra-

ation and severe accidents within the reactor coolant system and the spent fuel pool.

- COCOSYS, which is used for the detailed simulation of normal operation up to severe accidents within off-site release in the containment/buildings of LWR and limited capabilities for other reactor designs,
- NuT module (Numerical Toolkit), which provides an easy access to dedicated numerical libraries to speed up the internal computations of ATHLET and ATHLET-CD (ATHLET/CD). The focus currently lies on linear algebra subtasks.

ATHLET, ATHLET-CD and COCOSYS are one-dimensional lumped parameter codes. Each program has a modular structure and consists of several modules, which are described in detail in the following sections.

### 2.1 ATHLET

ATHLET [3] is composed of several basic modules for the simulation of the fundamental, multi-physical phenomena involved in the operation of a nuclear reactor, including thermal-fluid dynamics (TFD), heat transfer and heat conduction, neutron kinetics as well as control and balance-of-plant (see Fig. 2). Dedicated interfaces to external simulation tools such as 3D neutron kinetic codes, Computational Fluid Dynamics (CFD) codes or the AC<sup>2</sup> containment simulator COCOSYS are available. A flexible plug-in technique is used to couple user-provided code extensions.

The TFD-module of ATHLET offers two different sets of 1D model equations for the simulation of the fluid-dynamic behavior: A two-fluid model (6-equation model) with fully phase-separated conservation equations for liquid and vapor mass, momentum and energy, and a five-equation model with separate conservation equations for liquid and vapor mass and energy, supplemented by a mixture momentum equation. Both models account for thermal and mechanical non-equilibrium. The five-equation model includes a mixture level tracking capability to capture both dynamic motion of and two-phase processes at a horizontal phase interface in a verti-

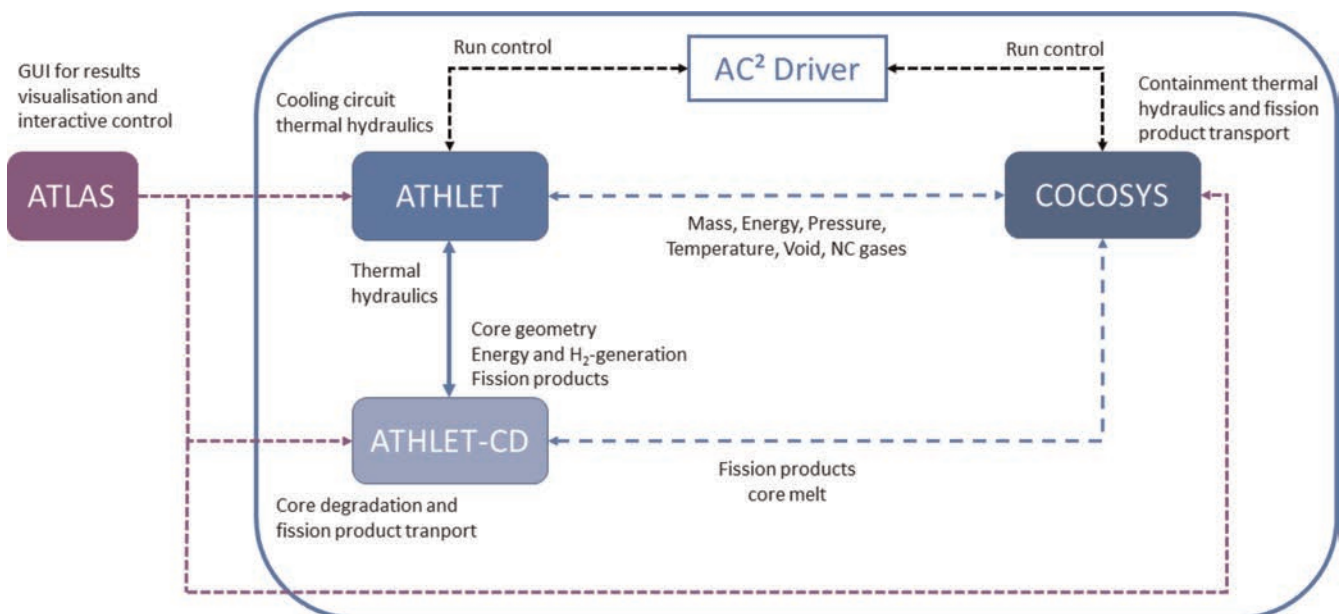


Fig. 1. Link between main modules of AC<sup>2</sup> (picture taken from [2])

cal component. A full-range drift-flux model is available for the calculation of the relative velocity between the fluid phases considering different geometries, such as horizontal pipes, vertical pipes, annuli or bundles. For the simulation of multidimensional, two-phase flow phenomena in large vessels such as the RPV, a 3D extension of the 1D two-fluid model is included.

The range of working fluids covers light and heavy water with consideration of the transition between subcritical and supercritical fluid states. In addition, helium, liquid sodium, lead and LBE (lead-bismuth eutectic) can be selected as coolant. These extensions aim at the simulation of future Generation IV reactor designs.

ATHLET also allows for the simulation of non-condensable gases. Fluid properties are provided for hydrogen, nitrogen, oxygen, air, helium and argon, but users can define their own non-condensable gases, if material properties are known. Additional balance equations can be included for the description of boric acid or zinc-borate transport within the coolant system as well as for the transport and release of nitrogen dissolved in the liquid phase of the coolant.

The heat transfer package (HECU) covers a wide range of single-phase and two-phase flow conditions. Correlations for critical heat flux (CHF) and minimum film boiling temperature are included. The influence of spacer grids on the CHF can optionally be considered. Evaporation and condensation directly at heating or cooling surfaces are calculated. A quench front model for bottom and top reflooding is also available. Special heat transfer correlations are available for supercritical water, liquid metal working fluids and helium, accounting for specific geometries such as rod bundles or pebble beds. ATHLET enables the simulation of two-dimensional heat conduction in structural components, for which either built-in or user-provided material properties can be used.

The time-dependent behavior of the nuclear power generation is calculated by a point-kinetics model. The point-kinetics model is based on the application of the kinetics equations for one group of prompt and for six groups of delayed neutrons. The reactivity changes due to control rod movement as well as reactivity feedback effects for fuel temperature, moderator density, moderator temperature and boron concentration are considered. For an in-depth analysis of core behavior, e.g. in case of asymmetric transients, ATHLET offers a general interface for coupling of 3D neutron kinetic models. Several 3D codes for rectangular and hexagonal geometries have

been successfully coupled to ATHLET (e.g. the GRS code QUABOX/CUBBOX or DYN3D by HZDR).

Specific models are provided for the simulation of valves, pumps, accumulators, heat exchangers, steam separators, steam and gas turbines, compressors, steam condensers, single and double ended breaks, fills and leaks.

The time integration of the thermo-fluid dynamic model is performed with a general purpose ordinary differential equation (ODE) solver. It provides the implicit solution of a linear system of ODE of first order. The linearization of the underlying conservation equation system is done numerically by calculation of the Jacobian matrix. A block sparse matrix package is available to handle in an efficient way the repeated evaluation of the Jacobian matrix as well as the solution of the resulting system of linear equations. For the very effective solution of the linear equation systems in the case of big simulation models a new software called NuT (see 2.4) can be used alternatively. A rigorous error control is performed using a higher order scheme for the time integration obtained by an extrapolation approach.

For the very important calculation of the leak mass flow, a special sub-program CDR1D is used. In contrast to commonly used methods like HEM or Moody (which are also offered by ATHLET) CDR1D calculates the leak mass flow by solving a 4-equation set of conservation equations in 1D. The specific geometry upstream of the leak can be provided by the user and is automatically discretized using a very fine nodalization, to be able to consider the very high velocity gradients near the leak.

ATHLET has been developed and validated to be applied for all types of design basis and beyond design basis incidents and accidents without core damage in LWR, like PWR, BWR, VVER, and RBMK.

## 2.2 ATHLET-CD

The module ATHLET-CD [4] covers the phenomena that are related to core degradation in a PWR, BWR or VVER type reactor. It has a modular structure and embeds ATHLET, which is used for the necessary thermohydraulic calculations (see Fig. 3).

Like other nuclear code systems, ATHLET-CD divides the core region radially into concentric rings and axially into different levels. It is assumed that all the fuel rods located in a user-defined ring behave identically which is a valid assumption.

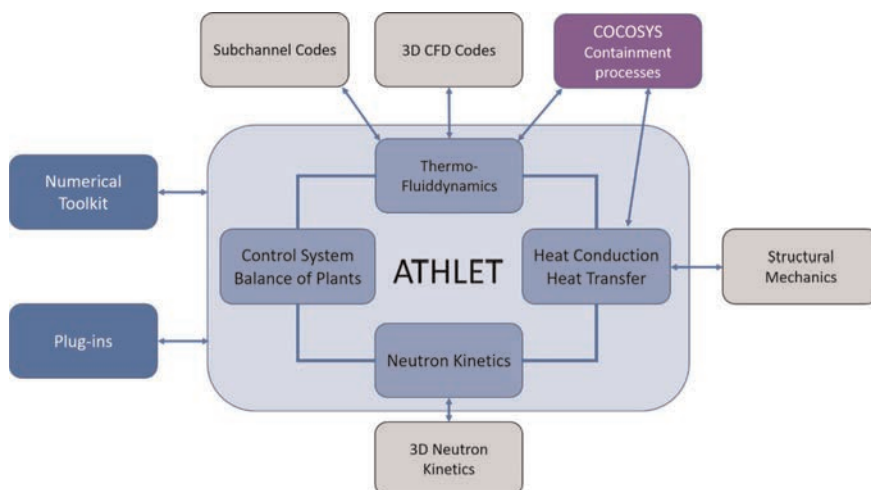


Fig. 2. Modular Structure of ATHLET [2]

tion if the analysed scenario is dominated by radially symmetric phenomena. An example of the core nodalization is shown in Fig. 4. The top view indicates that all fuel rods, which are located in one ring are combined and are visualized by one representative fuel rod, as depicted in the side view.

The submodule ECORE (see also code structure in Fig. 3) calculates core heat-up, oxidation effects and core degradation phenomena. Heat balance equations are solved for the fuel, for the absorber material, for the cladding and for the melt/crust. Blockage formation is considered during the melting processes.

The cladding oxidation model calculates the oxidation of zirconium and the associated hydrogen generation which is important to consider with increasing temperature of the core (above ~1000 K). Besides the oxidation in a steam environ-

ment, an approach is formulated to consider also nitride formation in an air environment. The parameters for the empirical correlations are determined based on single effect tests, see [5].

For the simulation of debris beds a specific model called MEWA is under development at IKE Stuttgart [6] with its own thermal-hydraulic equation system, coupled to the ATHLET-thermo-fluid-dynamics on the outer boundaries of the debris bed. The transition of the simulation of the core zones from ECORE to MEWA depends on the degree of degradation in the zone.

The fission/decay power of the reactor core can be defined via a time depending function or by using the FIPISO submodule. These submodules calculate the decay power and the fission product inventory after shutdown, using a user defined

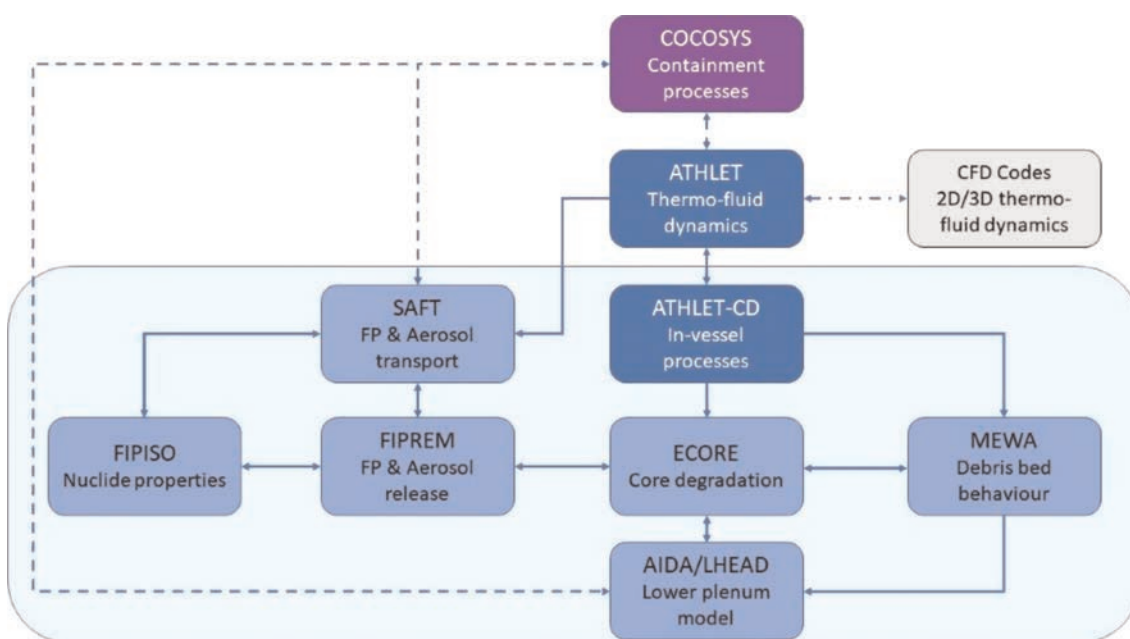


Fig. 3. Modular structure of ATHLET-CD (from [2])

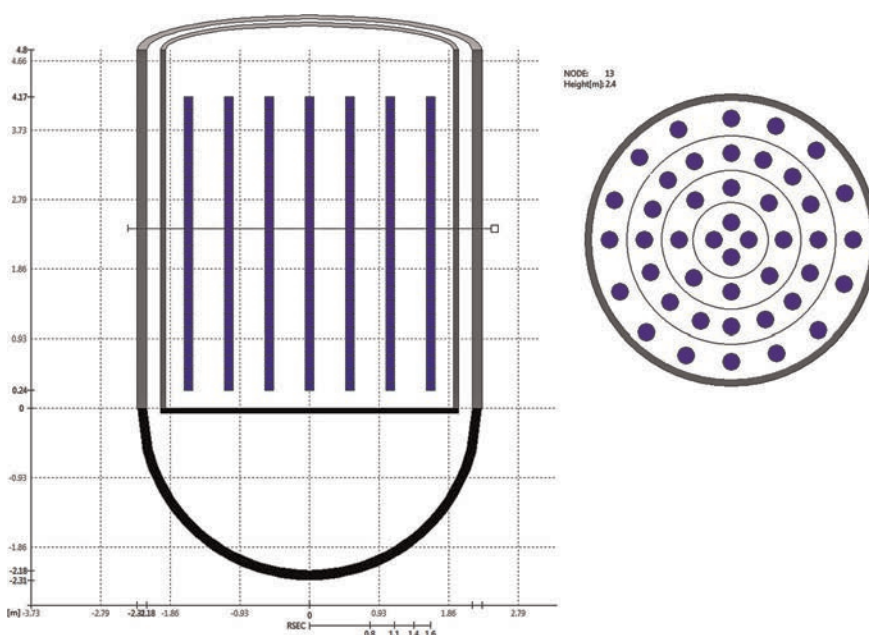


Fig. 4. Side and top view of the core nodalization in ATHLET-CD/AC<sup>2</sup> (from [4])

burn-up history and initial fissile material content of the core. The modules take 1296 isotopes separately into account using the appropriate property of each isotope.

The submodule FIPREM calculates the fission product release from the fuel rods. Fission product release is calculated if the cladding fails and the fuel temperature exceeds a user defined limit. Cladding failure criteria can be a constant parameter or a dedicated model, which constantly calculates the deformation of the cladding due to the heat up and oxidation. The release calculation is mainly based on the Antoine approach, where the release rate depends on the temperature of the fuel, system pressure and the partial pressure of the released material. For several relevant fission products that are sensitive to the oxidizing and reducing conditions the amount of available oxygen is also considered. The transport of these fission products and aerosols within the cooling circuit is calculated by the SAFT module based on the code SOPHAEROS [7].

The transported fission products are decaying during the transport and deposition, adding their power from alpha and beta decay to the surrounding structures or medium. The transport module takes a wide range of chemical and physical phenomena into account that influence the amount of fission product that reaches the containment:

- Agglomeration: the motion of aerosol particles leads to collisions and they stick together.
- Condensation on walls/aerosols: fission products released as vapors condense on colder structures or other aerosols.
- Sedimentation: due to gravity aerosols settle on horizontal surfaces.
- Turbulent impaction: Brownian motion of particles results in collision with and deposition at the wall.
- Bend impaction: the inertia of the particles causes in changes of system geometry deposition on walls.
- Thermophoresis: the particles with higher temperatures push the other particles towards colder regions, eventually causing deposition on wall.
- Diffusiophoresis: condensation of steam causes a flow of gas with particles towards walls.

These phenomena are also schematically depicted in (Fig. 5).

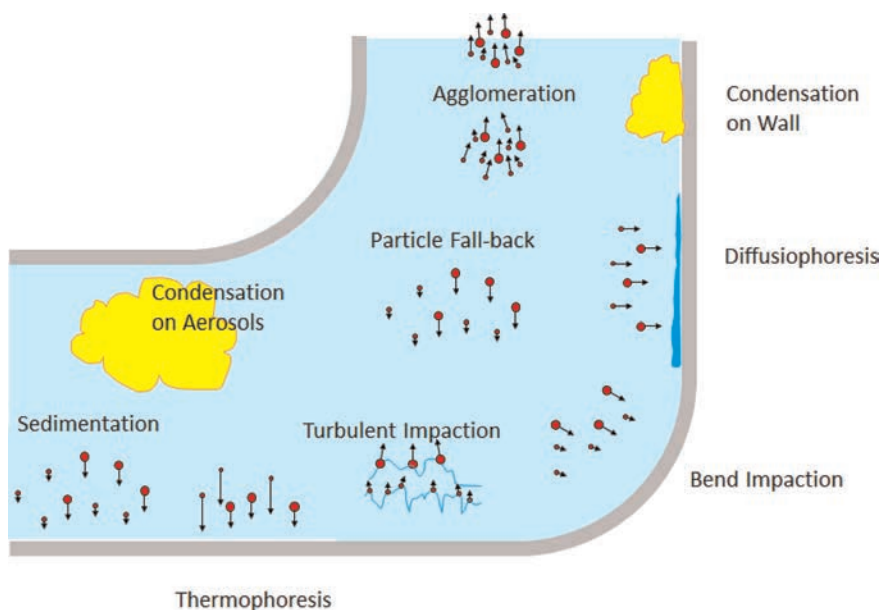


Fig. 5. Main phenomena in the fission product transport module in the reactor circuit of ATHLET-CD/AC<sup>2</sup>

Two modules are available to model the relocated molten material behaviour in the lower head: AIDA and LHEAD.

AIDA starts after the failure of the lower core grid plate (PWR) or after the failure of the control rod guide tubes (BWR). The relocation of the molten material from the core into the lower head is governed by ECORE and is not modelled in detail, yet. The molten material fills the lower head instantaneously at the beginning of the AIDA calculation. AIDA simulates the thermal behavior of the molten corium pool and the crust formation and the heat transfer through the crust and RPV wall. Heat conduction through the pressure vessel wall is solved two-dimensionally with a finite difference method. The corium pool is calculated with simplified, zero-dimensional balance equations, and additional empirical correlations are used to determine the heat fluxes. Homogeneous or stratified (two-layer) pool configuration models are available. The modelling of transient external reactor vessel cooling is possible with predefined or calculated heat transfer coefficients, considering also boiling conditions. AIDA is equipped with a wall-ablation model. Wall failure is predicted with a simple failure criterion considering the pressure difference, the temperature, the remaining wall thickness and the mass of the corium as well as the mass of the vessel wall under the corium pool. The transferred heat through the wall as well as the mass and energy data of corium after a vessel failure are provided to the containment code COCOSYS, if it is also activated.

The module LHEAD offers a more detailed nodalization of the lower head fluid domain and, thus, it allows the consideration of the lower head structures and the phenomena in the lower plenum. Especially for the simulation of late phase accidents in BWRs such detailed modelling is of interest to consider special structures like penetrations through the vessel (e.g. control rod guide tubes).

### 2.3 COCOSYS

COCOSYS [8] itself consists of the three separate main modules THY (THERmal HYdraulics), AFP (Aerosol and Fission Product behavior) and CCI (Core Concrete Interaction). Communication among these main modules is accomplished via MPI (Message Passing Interface), see Fig. 6.

### 2.3.1 Thermal Hydraulic (THY) Module

The thermal hydraulic (THY) module is a lumped-parameter model. The compartments of the considered containment or test facility must be subdivided into control volumes. The thermodynamic state of a zone is defined by its temperatures and masses of the specified components and the pressure. A few basic zone models are implemented in the THY main module of COCOSYS: an equilibrium and a non-equilibrium zone model and a pressure suppression zone model, among others. For the coupling to CFD codes an interface zone model may be utilized.

To describe the flow interaction between different zones, specific junction models are implemented, like rupture discs, atmospheric valves, flaps/doors or specific pressure relief valves used in Russian types reactors. The implemented pump system model is flexible enough to simulate complete cooling systems, e.g. containment spray systems or emergency core cooling systems.

Structure objects simulate walls, floors and ceilings of the containment. They can be partly submerged by water and can simulate various types of heat sinks within and between zones. The heat flux calculation is one-dimensional, solving the Fourier equation. The heat exchange between structures and assigned zones are calculated via convection, condensation and radiation. To consider condensate flows running along several structures, special flow paths can be defined and the water drip-off from structures can be simulated.

For the simulation of both design basis and severe accident sequences including possible accident management measures it is necessary to model hydrogen related phenomena and to

consider containment related safety systems. In the THY main module it is possible to simulate pump and spray systems, different types of coolers, ventilation systems and condensers. For simulation of Russian WWER and RBMK type containments, models are incorporated for specific safety flaps, weight dependent valves or U-shape hydro locks. Hydrogen recombination can be simulated by thermal recombiners as well as by passive autocatalytic recombiners (PARs).

A simplified model simulates hydrogen combustion and flame propagation between different compartments. It was validated against several hydrogen combustion experiments covering a broad spectrum of possible scenarios.

### 2.3.2 Aerosol and fission product (AFP) Module

The aerosol and fission product (AFP) main module is used for best-estimate simulations of the fission product behavior in the containment. Interactions between the thermal hydraulic and the aerosol and fission product behavior are considered via inter-model communication (see Fig. 6). The aerosol behavior of up to eight chemically different aerosol components is calculated with consideration of the thermal hydraulic boundary conditions. The module differentiates between soluble and insoluble as well as hygroscopic and non-hygroscopic aerosols. Sedimentation, diffusive deposition, thermophoresis and diffusio-phoresis are covered.

There are special models for the simulation of high-efficiency particulate air (HEPA) fibre and granulate filters implemented as well as an empirical model of a venturi scrubber type filter. The retention of aerosols during gas transport through water pools is calculated by the SPARC-B model.

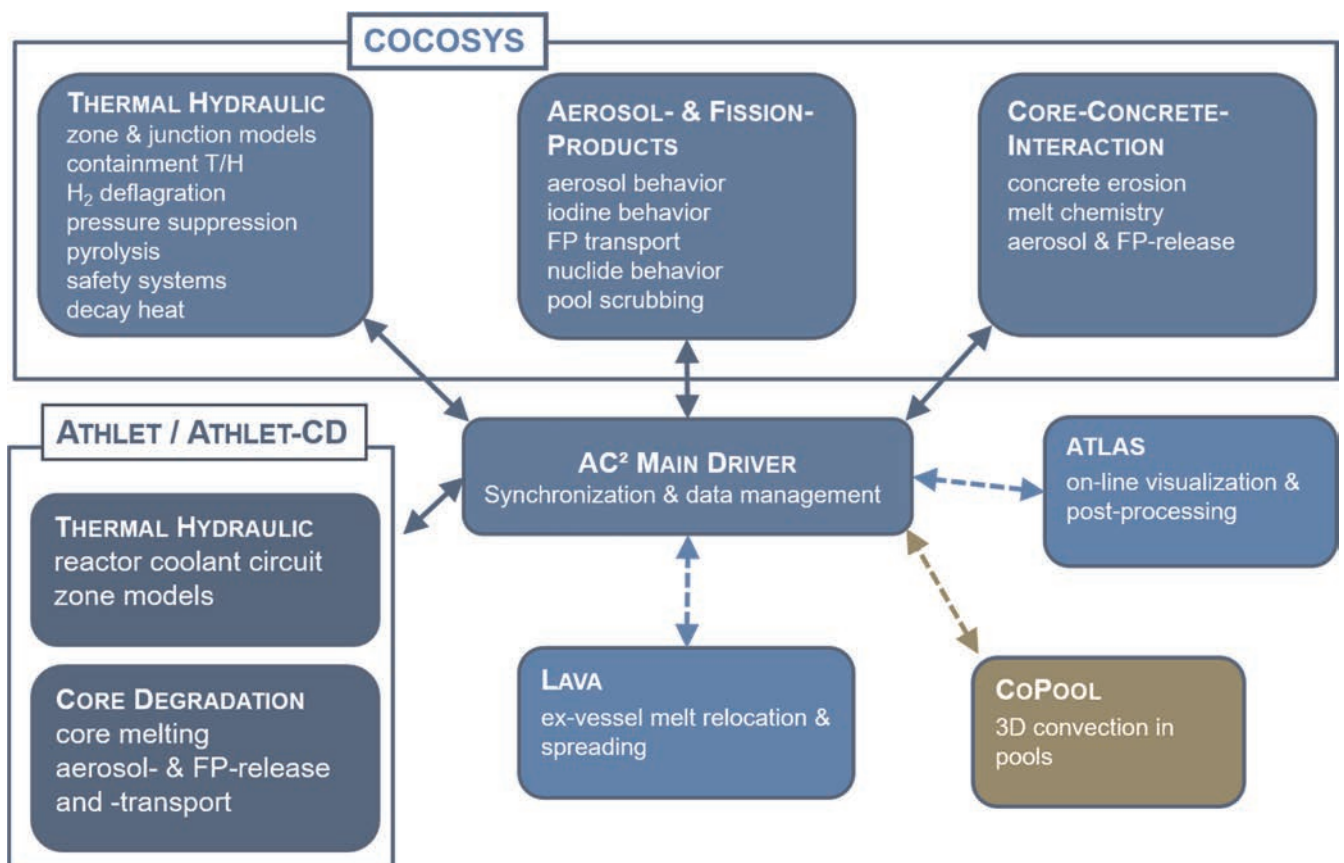


Fig. 6. Structure of COCOSYS code system (picture taken from [2])

This allows among other things the simulation of “pool scrubbing” in the pressure suppression system of a boiling water reactor.

For the simulation of the transport of the fission products it is differentiated between the atmosphere, the aerosol particles and the sump water as fission product carriers. The fission products can be deposited on surfaces in the atmosphere and in the sump. All relevant processes related with the fission products and the different carriers are considered: deposition of aerosol particles by natural processes or aided by technical systems such as retention in filters and wash-out by spray systems, washing-off from walls, and carrier change due to radioactive decay (see corresponding coefficients in Fig. 7).

The behavior of radioactive nuclides can be simulated with the help of the FIPISO model. It considers the reactor’s initial core inventory (up to 1296 isotopes) and calculates on this basis the decay of the relevant fission products according to the time of the onset of the release by using established nuclide libraries, no decay chains must be defined by the user.

The iodine chemistry is treated by the semi-mechanistic model AIM-3 (Advanced Iodine Model, 3rd version), which is and has been improved [9] according to the outcome of various THAI iodine [10] and other experiments. AIM-3 simulates in detail the transport and the behavior of iodine species in a multi-compartment geometry. It considers approx. 70 different reactions in the gas and in the water phase of a compartment. Also, the impact of engineered systems (filter, spray, etc.) on the iodine behavior is modelled.

### 2.3.3 CCI (Corium Concrete Interaction) Module

In the case of a failure of the reactor pressure vessel (RPV) the corium melt will be relocated into the containment cavity. The CCI module describes realistically the interactions of the

corium with the atmosphere and the structures in the containment considering:

- sources of thermal energy, fission products and non-condensable gases in the local corium pool
- melting of structural material and incorporation of molten material into the corium melt
- effect of deep-water layers in containment rooms on the coolability of the corium
- loss of containment integrity via melt-through
- melt relocations into other compartments within the containment

Corium ejection from the RPV under low pressure may lead to a significant pool of liquid corium in the cavity. In AC<sup>2</sup>/COCOSYS the same model basis as of ASTEC/MEDICIS [11] is used for the solution of mass and energy balances of a single corium pool under MCCI conditions. Homogeneous pools may evolve with time from the initial homogenous mixture to a stratified configuration of two layers. Fission product release from the MCCI pool is also considered. Generally, multiple melt pools (e.g. in different rooms) with interactions between molten corium and containment structures (sidewall, floor) may be defined.

Corium ejection from the RPV under elevated pressure leads to a considerable direct energy transfer from the finely distributed, gas-carried melt to the containment atmosphere, summarized under the acronym direct containment heating. Dedicated models are available for the relevant processes during this process. COCOSYS was applied to several integral direct containment heating experiments in the DISCO test facility in Karlsruhe. In the experiments, the reactor cavities of KONVOI, EPR and the French P’4 reactor types were modelled. Overall, compared with the measured data, satisfactory agreement of the integrally dispersed parts of the melt and of

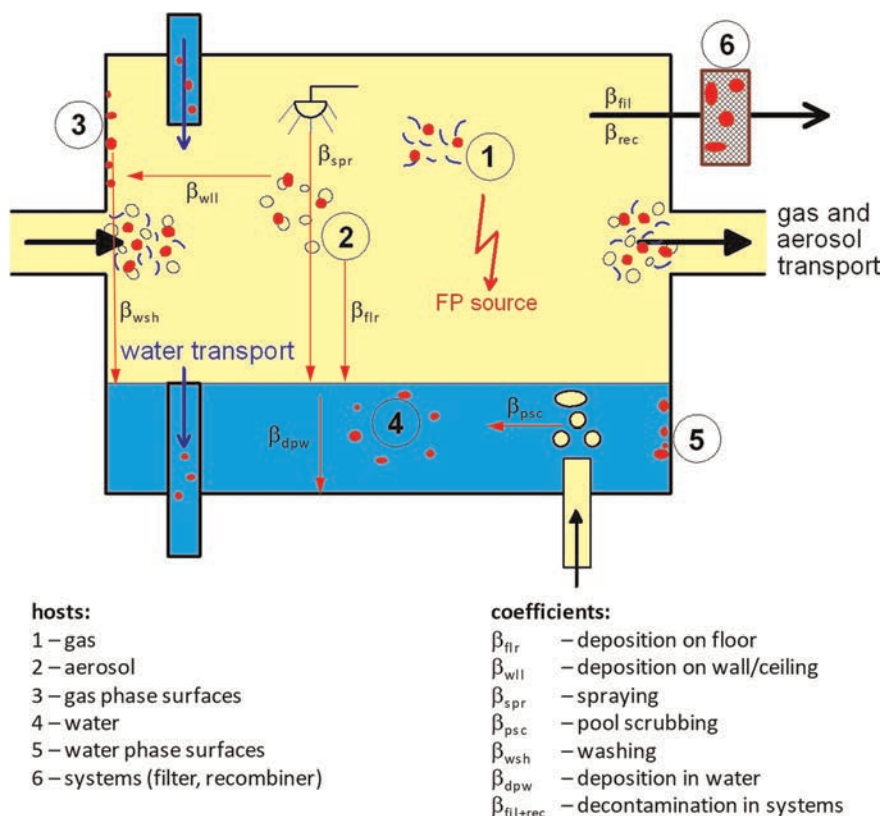


Fig. 7. Main aerosol and fission product phenomena simulated in COCOSYS/AC<sup>2</sup> (from [8])

the maximum pressures was achieved. Even “blind” calculations (i.e. without knowing the experimental results) showed a good prediction capability of the model, provided that empirical model parameters were adapted to other experiments using the same geometrical design, afore [12].

For the evaluation of the core catcher concept of the Generation 3+ EPR with view to corium spreading capabilities COCOSYS features a dedicated corium spreading model called LAVA [13].

#### 2.4 Numerical Toolkit (NuT)

A significant workload of the time integration process in ATHLET/ATHLET-CD relates to linear algebra tasks. This is especially true for large and/or complex problems with a considerable amount of cross-connections. Therefore, it is reasonable to make use of dedicated algorithms and data structures. The Numerical Toolkit (NuT) provides access to the third-party library PETSc [14, 15] which in turn may invoke the direct sparse solver MUMPS [16]. By means of these libraries the Numerical Toolkit defines several solver presets for the user to choose from to tackle the linear algebra in ATHLET/CD. Included are preconditioned iterative methods as well as direct methods. In contrast to ATHLET/CD's default numerics, scalable linear algebra algorithms and data structures are made available as well. This turns out to be of great benefit, especially in case of large problems, see [17].

Distributed computing and data storage in PETSc and MUMPS is established by the message-passing standard MPI. This standard is also used to manage the communication between ATHLET/CD and the Numerical Toolkit (see also Fig. 1). On the part of ATHLET/CD, communication is encapsulated in a plugin that may be invoked by ATHLET/CD of version 3.2 or higher.

#### 2.5 Coupling of AC<sup>2</sup> with external Codes

To allow multiphysical or multiscale simulations, AC<sup>2</sup> offers dedicated coupling interfaces to several specific computer codes. For the simulation of asymmetric transients, the 3D diffusion code neutron flux solvers QUABOX/CUBBOX by GRS and DYN-3D by HZDR can interact with AC<sup>2</sup>.

If some parts of the cooling system or the containment should be analyzed with explicit consideration of 3D phenomena in detail, an interface to the CFD-Codes ANSYS-CFX and OpenFOAM is available [3]. For a detailed subchannel simulation AC<sup>2</sup> offers an interface to COBRA-TF. Depending on the characteristic time constants of the coupled processes, the coupling techniques used range from weak form (e.g. data transfer after completed time step) to strong or semi-implicit form (i.e. mutual iteration of the codes' results for each substep of the AC<sup>2</sup> extrapolation algorithm, used for coupling with CFD codes).

Moreover, AC<sup>2</sup> can be extended by user provided feature implementations. A plug-in concept enables the user to extend AC<sup>2</sup> by user-defined-functions and models (e.g. own heat transfer correlations), which can be provided as shared libraries or DLLs.

#### 2.6 ATLAS

The visualization software ATLAS is a powerful postprocessing tool for the analysis of AC<sup>2</sup> results. But it can not only be used for postprocessing of AC<sup>2</sup> results but also for an interactive control of AC<sup>2</sup> simulations. This means that the user is not only able to start and stop a simulation of e.g. a nuclear

power plant, but also to open a leak, open or close valves, start or stop pumps and so on. ATLAS together with AC<sup>2</sup> therefore becomes a complete plant simulator, which can be used, for example, to test the effect of manual actions on the accident progression. The user interface of ATLAS is depicted in Fig. 8.

### 3 Quality Assurance

#### 3.1 Validation

To assure that a computer program produces reliable results, continuous and comprehensive verification and validation efforts are necessary. For AC<sup>2</sup> the whole spectrum of pre- and post-test calculations of separate effects tests, integral system tests including the major International Standard Problems, as well as real plant transients are used for code validation. The validation of AC<sup>2</sup> is based on the CSNI validation matrices for thermal hydraulic codes [18] and for containment codes [19]. According to GRS-internal QA-procedures these validation calculations against an experiment must be performed independent from the developer of the specific models. The validation of AC<sup>2</sup> is mainly done by GRS, see also the topical articles [20] and [21] on the validation of ATHLET/ATHLET-CD and COCOSYS. The following partners continuously support the development and validation of AC<sup>2</sup>: Ruhr Universität Bochum, Helmholtz Zentrum Dresden-Rossendorf, Hochschule Zittau Görlitz, TU München, Karlsruhe Institute of Technology (KIT) and the Institut für Kernenergetik und Energiesysteme (IKE) of the University Stuttgart.

The validation of the phenomena inside the cooling system was done for western light water reactors as well as for Russian type WWER reactors. The simulated test cases covered the whole accident spectrum from small, medium and large break LOCAs and transients for pressurized water reactors as well as for boiling water reactors. Among others, test data of the facilities LOFT, LSTF, BETHSY, PKL, SPES, LOBI, UPTF, TRAM are used in the validation process.

In the case of severe accidents special emphasis is laid on the validation of the models for bundle degradation as well as release and transport of fission products and aerosols. Amongst others, test data of QUENCH, PHEBUS and LIVE facilities were used. For validation of severe accident simulation of a whole plant the TMI accident is an important reference case.

The simulation of the phenomena inside the containment is validated on a wide spectrum of separate and integral experiments performed at German and international test facilities. The experiments performed in the former Battelle Model Containment (BMC) and the former Heiß-Dampf-Reaktor (HDR) as well as the ongoing tests in the THAI facility represent a strong pillar of the COCOSYS validation. The CCI module is validated based on experiments selected from the ACE, OECD-CCI and MOCKA test series. Furthermore, for the simulation of all AC<sup>2</sup> components, GRS uses results of their participation in several international experimental research programs (OECD THAI/BIP/STEM, PKL, ...).

In the last years, one focus for the validation of AC<sup>2</sup> was the simulation of passive safety systems of Generation 3/3+ reactors. As one reference for the validation of AC<sup>2</sup> the KERENA reactor concept design is used as it utilizes several advanced safety systems like emergency condensers, passive heat exchangers, suppression and flooding pools, and as the INKA test facility operated at AREVA offers unique experimental results for code validation [22]. Comparable passive system concepts are also used in other Generation 3/3+ de-



signs as AP1000 and CAP1000. The INKA test set-up allows testing of single components and integral system testing. As the facility is full scale and full pressure and comprises the cooling system and the containment it is possible to simulate accident scenarios with realistic boundary conditions.

### 3.2 Continuous integration

For the automatic verification and validation of AC<sup>2</sup> a continuous integration platform based on the software Jenkins [23] is used [24]. It automates different steps of the verification and validation process. After every commit of new or changed code to the source code management system, the software is built for all supported operating systems and configurations. To check that the new or changed code has no unwanted effects several unit test and verification and validation tests are executed. Different sets of tests are performed on different schedules, simple tests cases are run daily, more challenging tests use a weakly test pipeline. If the results of these tests show deviations from the specified test targets, immediate actions can be taken to resolve any problems. This procedure of a continuous integration has helped to improve both the quality of the software and productivity.

### 4 Current and future goals of the AC<sup>2</sup> development

One important topic of the current further development of AC<sup>2</sup> are passive safety systems. As most of these systems

work at low pressures, AC<sup>2</sup> will get a new water/steam property package with a very precise calculation of the data particularly at low pressures. This package will be first available in ATHLET. Moreover, the correlations used for heat transfer coefficient calculation are checked for their appropriateness for passive systems. Further the flow regime maps are overworked. COCOSYS will come with a new fission product transport module in the next version. Besides the melt behavior is improved, more precisely the underwater spreading and the behavior in a core catcher. In ATHLET-CD a more flexible core nodalization scheme with radial and azimuthal relocation of melt is under development. The numerical toolkit NuT, which works only for ATHLET calculations in the current version, will be available also for COCOSYS and coupled simulations in future. For AC<sup>2</sup> the coupling abilities between the modules are further improved, especially made more flexible. To make AC<sup>2</sup> more user-friendly, the input needed for coupled calculations will be easier to build up.

### 5 Summary

The program package AC<sup>2</sup> consisting of the modules ATHLET, ATHLET-CD and COCOSYS is suitable for the simulation of all conditions of normal operation, operational occurrences, design basis accidents and severe accidents for a broad spectrum of light water-cooled reactors of Generation 2,3/3+. The thermohydraulic system code ATHLET uses a six equation two fluid model together with a multitude of spe-

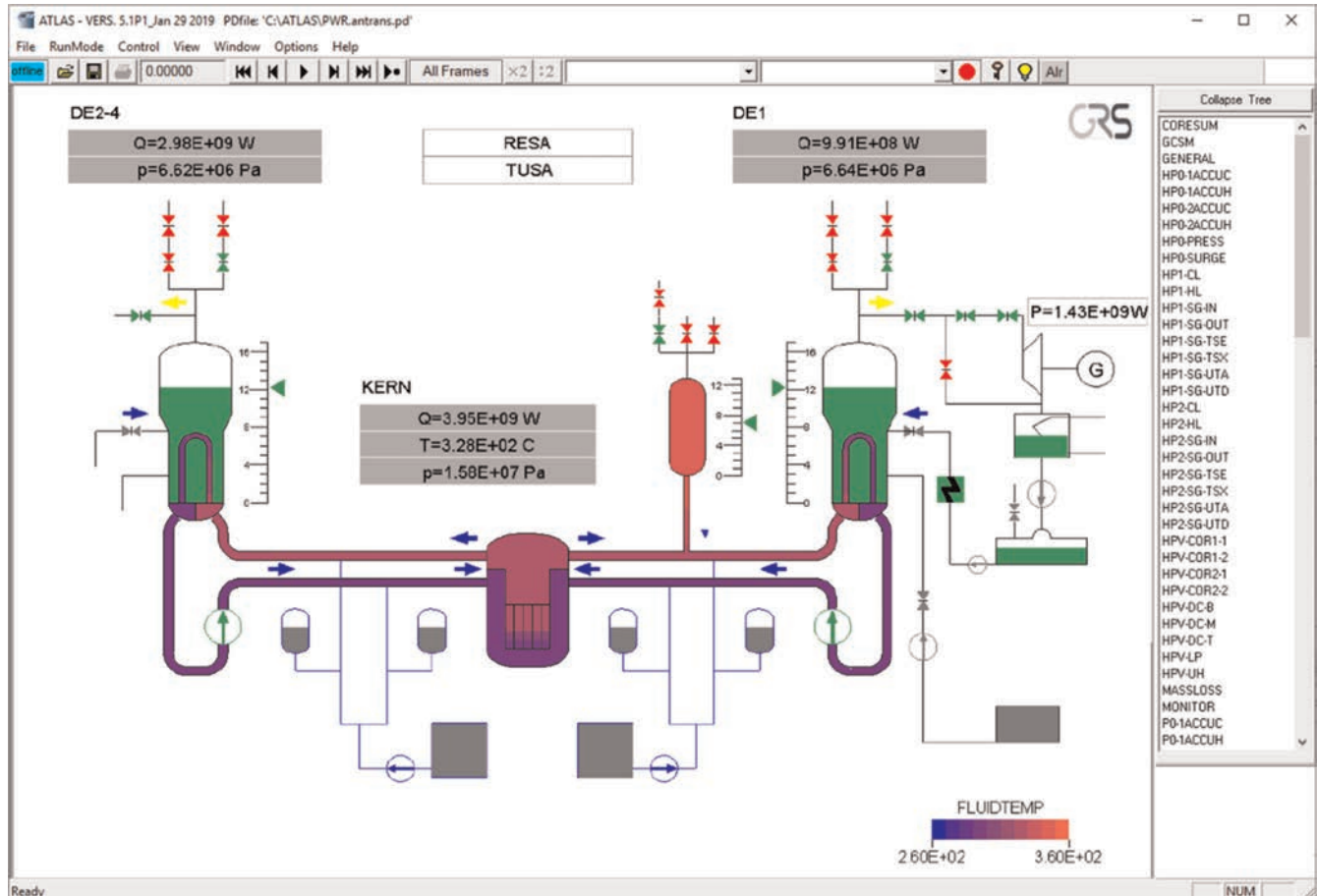


Fig. 8. ATLAS user interface for postprocessing and interactive control of AC<sup>2</sup> simulations (GRS)

cial component models to simulate all phenomena inside the primary and secondary cooling system. ATHLET-CD extends ATHLET for the simulation of accidents with core degradation. The containment code COCOSYS calculates the containment behavior under design basis accidents and phenomena like fission product spreading and melt behavior under accident condition. The common AC<sup>2</sup> driver for all modules allows not only for standalone calculations of the single modules, but also for coupled calculation. Especially for Generation 3+ plants this code feature to couple the cooling circuit with the containment is very important. This enables the simulation of the whole passive cooling chain transporting the residual heat from the core through the cooling circuit to the containment and finally to the environment. The further improvement of AC<sup>2</sup>'s ability to simulate passive safety system is one of the main working topics in the next years.

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### The authors of this contribution

Fabian Weyermann (corresponding author),  
Claus Spengler, Philip Schöffel, Sebastian Buchholz, Tim Steinhoff,  
Martin Sonnenkalb, Andreas Wielenberg, Andreas Schaffrath  
E-mail: Fabian.Weyermann@grs.de  
Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH,  
Schwertnergasse 1, 50667 Cologne (DE)

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