Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

# ATHLET 3.4

## Program Overview

November 2023

AC²
ATHLET

# 1 Overview of ATHLET

The thermal-hydraulic computer code **ATHLET** (**A**nalysis of **TH**ermal-hydraulics of **LE**aks and **T**ransients) is being developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (**GRS**) for the analysis of operational conditions, abnormal transients and all kinds of leaks and breaks in nuclear power plants. The aim of the code development is to cover the whole spectrum of design basis and beyond design basis accidents (without core degradation) for **PWRs, BWRs, SMRs and future Gen IV reactors** with one single code.

The main code features are:

- advanced thermal-hydraulic modelling (compressible fluids, mechanical and thermal non-equilibrium of vapor and liquid phase)
- availability of diverse working fluids: light or heavy water, helium, sodium, potassium, lead or lead-bismuth eutectic, supercritical carbon dioxide, molten salts as well as user-provided single-phase (non-boiling) working fluids
- heat generation, heat conduction and heat transfer to single- or two-phase fluid considering structures of different geometry, e.g. rod or pebble bed
- interfaces to specialized numerical models such as 3D neutron kinetic codes or 3D CFD codes for coupled multiphysical or multiscale simulations
- control of ATHLET calculation by call backs to programming language independent user code enabling the coupling of external models
- plug-in technique for user provided code extensions
- modular code architecture
- separation between physical models and numerical methods
- numerous pre- and post-processing tools
- portability
- continuous and comprehensive code validation

ATHLET is applied by numerous institutions in Germany and abroad.

The development and validation of ATHLET is funded by the German Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection (BMUV) based on decisions by the German Bundestag.

## 1.1 Range of Applicability

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 light water reactors, like PWR, BWR, VVER, and RBMK. For accidents with core damage, **ATHLET-CD** (**C**ore **D**egradation) has been developed providing extensions for the simulation of the mechanical fuel behaviour, core melting and relocation, debris bed formation as well as fission product release and transport within the reactor system. ATHLET-CD uses the same input deck as ATHLET supplemented by data required by the core degradation models.

The range of working fluids covers **light and heavy water** enabling the transition between subcritical and **supercritical fluid states**. In addition, further coolants can be simulated as working fluids: **helium, sodium, potassium** as well as **non-boiling fluids liquid lead, lead-bismuth eutectic, molten salts** and **user-provided fluids**. These extensions, aiming at the simulation of future Generation IV reactor designs, are still subject to further development and validation.

ATHLET is a 1D system code, ATHLET is not a 3D CFD code. ATHLET thermal hydraulic models generally assume fully developed flow on dimensions (0.01 m to 10 m) and pressures (0.01 MPa to 30 MPa) typical of nuclear facilities. Details of turbulence, of boundary layer, and viscous energy dissipation between flow layers are neglected, interfacial area and momentum terms are treated in a simplified manner, and 3D flow effects cannot be investigated in detail. Similarly, heat conduction in structures generally is 1-dimensional using averaged, engineering level heat transfer correlations. While ATHLET can be applied outside of these constraints with some success, it has not been validated for them.

## 1.2 Code Structure

ATHLET is written in Fortran. The code features a modular code structure that allows an easy maintainability and expandability of the modelling basis to satisfy the demands of

new applications and future reactor designs. The code is composed of four basic modules that focus on the calculation of phenomena relevant for safety analyses of a nuclear power reactor:

- Thermo-Fluid dynamics (TFD)
- Heat Conduction and Heat Transfer (HECU)
- Neutron Kinetics (NEUKIN)
- Control and Balance of Plant (GCSM)

The TFD system of ordinary differential equations is solved fully implicitly with the numerical integration method FEBE. Other independent modules (e.g. large models with own time advancement procedure) can be coupled without structural changes in ATHLET by means of dedicated interfaces.

## 1.3 Fluid Dynamics

The TFD module of ATHLET employs a modular network approach for the representation of a thermal-hydraulic system. A given system configuration can be simulated just by connecting basic fluid dynamic elements, called **thermo-fluid dynamic objects (TFOs)**. There are several TFO types, each of them is applied with a selected fluid dynamic model. All object types are classified into three basic categories:

- **Pipe objects** employ a one-dimensional TFD model describing the transport of fluid. After nodalization according to input data, a pipe object can be understood as a number of consecutive nodes (**control volumes**) connected by flow paths (**junctions**). A special application of a pipe object, called single junction pipe, consists of only one junction, without any control volumes.
- **Branch objects** consist of only one control volume. They employ a zero-dimensional TFD-model of non-linear ordinary differential equations or algebraic equations.
- **Special objects** are used for network components that exhibit a complex geometry, e.g. the cross connection of pipe objects aligned in parallel for the generation of a multidimensional network.

This object structure has been developed in order to allow the coupling of models of different physical formulation and spatial discretization, which are to be employed in certain network domains.

ATHLET offers two different sets of model equations for the simulation of the fluid-dynamic behaviour:

- The **5-equation model** with separate conservation equations for liquid and vapor mass and energy, supplemented by a mixture momentum equation. It accounts for thermal and mechanical non-equilibrium and includes a mixture level tracking capability.
- The **Two-fluid model** with fully phase-separated conservation equations for liquid and vapor mass, energy, and momentum (without mixture level tracking capability).

The spatial discretization is performed on the basis of a **finite-volume staggered-grid approach**. The mass and energy equations are solved within control volumes, and the momentum equations are solved over junctions connecting the centres of the control volumes. The solution variables are the pressure, vapor temperature, liquid temperature and vapor mass quality within a control volume, as well as the mass flow rate (5-eq. model) or the phase mass velocities (6-eq. model) in a junction, respectively.

Two types of control volumes are available. Within the so-called “ordinary” control volume, a homogeneous mass and energy distribution is assumed. Within the “non-homogeneous” control volume, a **mixture level** is modelled. Above the mixture level, steam with water droplets, below the mixture level, liquid with vapor bubbles may exist. The combination of ordinary and non-homogeneous control volumes provides the option to simulate the motion of a mixture level through vertical components.

A full-range **drift-flux model** is available for the calculation of the relative velocity between the fluid phases. The model comprises all flow patterns from homogeneous to separated flow occurring in vertical and horizontal two-phase flow. It also takes into account counter current flow limitations in different geometries.

Moreover, both fluid-dynamic options allow for the simulation of **non-condensable gases**. This applies for water as well as for the liquid metal and molten salt working fluids. Fluid properties are provided for hydrogen, nitrogen, oxygen, air, helium, argon, krypton,

xenon, carbon monoxide, and carbon dioxide. Additional mass conservation equations can be included for the description of **boric acid** or **zinc borate** transport within a coolant system as well as for the transport and release of **nitrogen dissolved** in the liquid phase of the coolant.

Both the 5-equation model and the two-fluid model employ the one-dimensional conservation equations for mass, momentum and energy. By means of a spatially two- or three-dimensional TFO arrangement, these models allow for a simplified multidimensional simulation. In order to enhance the capability of ATHLET with regard to the simulation of complex, multidimensional flow phenomena, a **thermal-hydraulic 2D/3D model** has been developed. It extends the balance equations of the two-fluid model. Both 2D and 3D momentum equations for liquid and vapor are available.

For pipe objects applying the 5-equation model, there is also the possibility to use the method of integrated mass and momentum balances (**EIMMB**), an option for fast-running calculations, mainly in the frame of a nuclear plant analyser. With the application of the EIMMB-Method, the solution variables are now the average object pressure, the mass flows at pipe inlet and outlet, and the local qualities and temperatures. The local pressures and mass flow rates are obtained from algebraic equations as a function of the solution variables.

Another fluid-dynamic option, applied exclusively for the steady state calculation, consists of a 4-equation model with balance equations for liquid mass, vapor mass, mixture energy and mixture momentum. The solution variables are the pressure, vapor mass quality and enthalpy of the dominant phase within a control volume, and the mass flow rate in a junction. The entire range of fluid conditions, from subcooled liquid to superheated vapor including thermal non-equilibrium is taken into account, assuming the non-dominant phase to be at saturation.

## 1.4 Numerical Methods

The **time integration** of the thermo-fluid dynamic model is performed with the general-purpose ODE-solver **FEBE** (Forward-Euler, Backward-Euler). It provides the solution of a linear system of ordinary differential equations (ODE) of first order, splitting it into two subsystems, the first being integrated explicitly, the second implicitly. Generally, the **fully**

**implicit** option is used in ATHLET. Each thermo-fluid dynamic object provides a subset of the entire ODE system, which is integrated simultaneously by FEBE.

The linearization of the underlying model equation system is done numerically by calculation of the Jacobian matrix. A **block sparse matrix package** (FTRIX) is available to handle the repeated evaluation of the Jacobian matrix as well as the solution of the resulting system of linear equations in an efficient way. Alternatively, scalable solvers from the PETSc and MUMPS libraries can be used for the numerical calculations via the Numerical Toolkit (NuT) plug-in.

A **rigorous error control** is performed based on an extrapolation technique. According to the error bound specified by the user, the time step size and the order of the method (> 2) are adequately determined by FEBE for every integration step.

## 1.5 Heat Conduction and Heat Transfer

The simulation of the heat conduction in **structures, heat exchangers, fuel rods, electrical heaters and spheres** (pebble bed) is performed by the basic module **HECU**. It permits the user to assign heat conduction objects (HCOs) to all thermal-fluid dynamic objects of a given network.

The one-dimensional heat conductor module HECU provides the simulation of the temperature profile and the energy transport in solid materials. The model has the following characteristics:

- The shape of a HCO is constant in time.
- The model can simulate the one-dimensional temperature profile and heat conduction in plates normal to the surface, as well as in hollow or full cylinders and spheres in the radial direction.
- Optionally, two-dimensional heat conduction can be simulated considering the axial direction of plates and cylinders.
- In each HCO, up to three material zones can be modelled. A material zone is simulated by a user-defined number of temperature layers. The material zones can be separated by a geometrical gap and a corresponding heat transfer coefficient.

Furthermore, the model enables the calculation of the temperature in TRISO coated particles.

- The HCOs can be coupled on left and/or right side to TFOs by consideration of the energy transport between heat conductor surface and the surrounding fluid. It is also possible to simulate a fluid temperature as boundary condition for the HCO by means of control (GCSM) signals.
- The HCOs are automatically split into heat conduction volumes (HCVs) according to the nodalization of the adjacent TFOs and to user input.
- Heat generation can be considered in material zones. The specific heat generation rate per volume unit is assumed to be distributed uniformly either within a material zone or a temperature layer.
- Radiation heat transfer between different HCOs can be taken into account.

The **heat transfer package** covers a wide range of single phase and two-phase flow conditions of water. Correlations for critical heat flux and minimum film boiling temperature are included. 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 considering specific geometries (e.g. rod bundle or pebble bed).

## 1.6 Nuclear Heat Generation

The nuclear heat generation is generally modelled by means of the neutron kinetics module **NEUKIN**. For the simulation of electrically heated rods or for a simplified, straight-forward representation of a reactor core, the total generated power as a function of time or any other quantity can optionally be given.

The generated **nuclear reactor power** consists of two parts: the prompt power from fission and decay of short-lived fission products, and the decay heat power from the long-lived fission products. The steady state part of the decay heat and its time-dependent reduction after a reactor scram are provided in form of a GCSM signal. The time-dependent behaviour of the prompt power generation is calculated either by a point-kinetics model or by coupling to a 3D neutron kinetics code. An input-specified fraction of the total power is assumed to be produced not in the fuel but directly in the coolant.

The **point-kinetics model** is based on the application of the well-known kinetics equations for one group of prompts and for six groups of delayed neutrons. The reactivity changes due to control rod movement or reactor scram are given by a GCSM signal. The reactivity feedback effects for fuel temperature, moderator density and moderator temperature are calculated either by means of dependencies given by input tables or with reference reactivity coefficients. If the boron tracking model is applied, the reactivity feedback due to changes in the boron concentration will be also taken into account.

The module NEUKIN also offers a general interface for coupling of **3D neutronic models**. Several 3D codes for rectangular and hexagonal geometries have been successfully coupled to ATHLET with this interface, e.g. FENNECS; QUABOX/CUBBOX, TORT-TD, PARCS or DYN3D.

## 1.7 Simulation of Components

Specific models are provided for the simulation of **valves, pumps, accumulators, steam separators, steam and gas turbines, compressors, steam condensers, single and double ended breaks, fills, leaks, and boundary conditions** for pressure and enthalpy. The steam separator model is an empirical approach for the calculation of carry-over and carry-under flows by means of input functions of the inlet mass flow rates, of the void fraction in the separator region, and of the mixture level outside the separator. Abnormal separator conditions like flow reversal or flooding can be simulated.

In general, major plant components (e.g., pressurizer, steam generators) can be modelled by connecting thermo-fluid dynamic objects (TFOs) and heat conduction objects (HCOs) via input data. For compact heat exchanger designs like plate heat exchanger or helical coil heat exchanger dedicated models are available.

**Critical flow**, e.g. **discharge flow**, is calculated by a one-dimensional thermal non-equilibrium model with consideration of the given flow geometry. The module CDR1D generates automatically tables of critical mass fluxes applied in ATHLET for the interpolation of the critical mass flow rates. Optionally, a homogeneous equilibrium model and the Moody discharge model are available.

## 1.8 Simulation of Control and Balance-of-Plant

The simulation of balance-of-plant (BOP) systems within ATHLET is performed by the basic module **GCSM** (General Control Simulation Module). GCSM is a block-oriented simulation language for the description of control, protection and auxiliary systems.

The user can model control circuits or even simplified fluid systems just by connecting basic functional blocks (e.g. switch, adder, integrator). Most of the system variables calculated within the fluid dynamics, neutron kinetics or within other ATHLET modules can be selected as input to these functional blocks (process variables). The output of such control blocks can be fed back to the thermo-fluid dynamics in form of hardware actions (e.g. valve cross sectional area, control rod position) or boundary conditions (e.g. temperature, heat and mass sources).

The GCSM module allows for the representation of fluid dynamic systems (e.g. steam line, condensate system) in a very simplified way (quasi stationary approach) with the advantage of requiring very little computing time in comparison with the fluid dynamics module.

GCSM also provides an interface to a library that contains detailed models with fixed structure and own input data for plant components (e.g. heat exchanger or even containment model) or for control systems (e.g. power control or system pressure control for typical power plants).

The **GRS containment codes CONDRU and COCOSYS** have been coupled to ATHLET by means of this interface. In addition, GCSM comprises a flexible interface that enables the coupling of ATHLET with user provided code, that implements external models, new controller types, specific signals, or complete BOP models.

## 1.9 Code Handling

ATHLET provides a free-format, hierarchically structured input. Both the generation and the maintenance of the ATHLET input decks are facilitated by several copy functions and by the use of a flexible parameter technique during input data processing, which helps to avoid the repeated typing of identical or similar input data and adaptation of existing inputs to different configurations. An extended checking of both the input data and the

program processing helps the user to discover input errors or modelling weaknesses affecting both code performance and physical results.

ATHLET provides a **restart capability**. The program execution can be **parallelized** on computers with shared memory architecture using the Fortran OpenMP standard. ATHLET runs under different computer operational systems (MS Windows ®, Linux).

The ATHLET Program Package comprises a series of **auxiliary programs** to support both the ATHLET users and developers in the application and development of ATHLET:

- AGM: **A**THLET **G**CSM **M**odeler for graphical setup and testing of control systems and generation of GCSM input data.
- AIG: **A**THLET **I**nput **G**raphics for graphical representation of the TFO and HCO network specified in the input model.
- GIG: **G**CSM **I**nput **G**raphics for graphical representation of the structure of GCSM controllers.
- Several programs for the post-processing of plot data (concatenation, merging, algebraic operations, ...)
- ATLAS: Dynamic visualization of the simulation results on the basis of AIG and GIG pictures.
- Several programs for the analysis of the Jacobian matrix (interdependencies, Eigenvalues, …), mainly for code development and debug purposes.
- Furthermore, ATHLET can be applied as process model of the **ATLAS/ATLASneo plant simulator** providing full interaction and extended data visualization. ATLAS and ATLASneo are also components of the AC² software package.

ATHLET is also closely linked with the GRS computer programs **SUSA** and **MCDET**. Both enable uncertainty and sensitivity analyses of ATHLET simulation results.

## 1.10 Code Coupling

ATHLET is part of the **AC² software package**, which comprises the GRS codes ATHLET, ATHLET-CD and COCOSYS, includes the 3D nodal neutronics code FENNECS and is

complemented by the interactive simulator software ATLAS/ATLASneo and some productivity tools.

To allow **multiphysical or multiscale simulations**, ATHLET has been coupled successfully to various computer codes by means of dedicated coupling interfaces. The following figure depicts the essential interfaces that are realized for ATHLET. 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 sub step of the FEBE extrapolation algorithm, used for coupling with CFD codes).

Moreover, ATHLET can be extended by user provided feature implementations. The **plug-in concept** enables the users to apply ATHLET more individually by either requesting a specific extension from GRS or even by developing the needed feature on their own. Such plug-ins have to be created as separate shared libraries on Linux systems or DLLs under Windows. In case a plug-in binary is placed within the *plugin* directory of an ATHLET installation, ATHLET will register it at start up and invoke it if the applied input file demands its use. The parts or phases of the simulation that can be extended by plug-ins are specified by ATHLET.

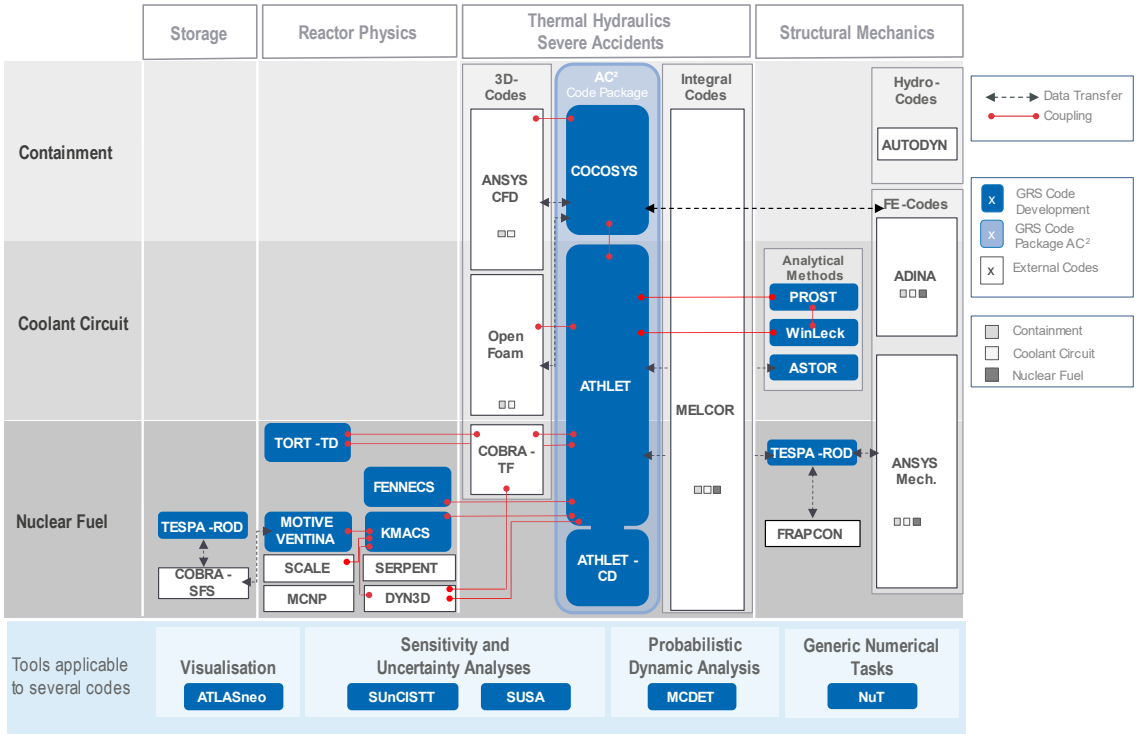


**Fig. 1.1** GRS nuclear simulation chain and code coupling

Another option for controlling the simulation by user code is offered by using the shared library version (MS Windows: dll / Linux: so) of ATHLET. This library provides the main entry of ATHLET via the exported routine symbol athlet_. This variant allows to implement a user program that calls ATHLET as a subroutine. In this case the simulation process can be controlled in an *"event oriented"* manner by associating the so-called **call back routines** before calling ATHLET. An *event* can be considered as a certain and named point in the simulation flow, like *input done*, *begin of timestep*, *end of timestep*. These points have been made available as the so-called **hooks**, at which a user might associate routines that instruct ATHLET what to do at this point before continuing the simulation. Hash maps, which include pointers to exported ATHLET variables, are accessible by both the user code and ATHLET. They enable inter-code data transfer of e.g., physical fields or GCSM control block states.

## 1.11 Validation

The development of ATHLET was and is accompanied by a systematic and comprehensive validation program. The validation is mainly based on pre- and post-test calculations of

separate effects tests, integral system tests including the major **International Standard Problems**, as well as on actual plant transients. A well-balanced set of tests has been derived from the **CSNI Code Validation Matrix** emphasizing the German combined ECC injection system. The tests cover phenomena which are expected to be relevant for all types of events of the envisaged ATHLET range of application for all common LWRs including advanced reactor designs with up-to-date passive safety systems, spent fuel pool applications as well as research reactors. The validation of ATHLET for SMR designs and future Gen IV reactors is underway.