Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

ATHLET

User's Manual

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Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

ATHLET 3.5

User's Manual

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Contents of User's Manual

This User's Manual comprises five parts:

- Part 1: ATHLET Description
- Part 2: ATHLET Input Data Description
- Part 3: ATHLET Variables Description
- Part 4: Support Software Description
- Part 5: Output Description

Detailed lists of contents can be found at the beginning of each part.

Acknowledgements

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Over the more than 40 years of continuous development on ATHLET and its predecessors, a very large number of people, both former GRS employees as well as external developers have contributed to the current status of ATHLET. Here, we want to acknowledge the work of those developers who have made major contributions to ATHLET in the past: Henrique Austregesilo, Christine Bals, Maria Burwell, Helmuth Deitenbeck, Ursula Gaal, Wolfgang Hobbhahn, Eduard Hofer, Adela Hora, Antoine Langenfeld, Jaejin Lee, Georg Lerchl, Wolfgang Luther, Dieter Loy, Christoph Müller, Juán E. Miró, Pavlos Papadimitriou, Winfried Pointner, Peter Romstedt, Johann-Dietrich Schubert, Tomasz Skorek, Heinz-Günther Sonnenburg, Fritz Steinhoff, Klaus Trambauer, Thomas Voggenberger, Klaus Wolfert. In addition, we would like to thank the teams from Hochschule Zittau-Görlitz (HSZG), Institute of Nuclear Technology and Energy Systems of University of Stuttgart, Ruhr-Universität Bochum (AG Plant Simulation and Safety, PSS) and Helmholtz-Zentrum Dresden-Rossendorf (HZDR) for their valuable contributions to the ATHLET code development and validation.

Finally, this code documentation profited from the support and contributions of Jennifer Born and Sandra Böhm in layouting, formatting and proofchecking the texts.

Preface

This User's Manual has been prepared to assist users in the effective application of the ATHLET computer code. ATHLET is an advanced best-estimate system code which has been initially developed for the simulation of design basis and beyond design basis accidents (without core degradation) in light water reactors, including VVER and RBMK reactors. Furthermore, this program version enables the simulation of further working fluids like helium, liquid metals, or molten salts.

The one-dimensional, two-phase fluid dynamic models are based on a five-equation model supplemented by a full-range drift-flux model, including a dynamic mixture-level tracking capability. Moreover, a two-fluid model based on six conservation equations is provided. The heat conduction and heat transfer module allows a flexible simulation of fuel rods and structures. Nuclear heat generation is calculated by a point-kinetics model or with a coupled 3D neutron kinetics code. A general control simulation module is provided for flexible modelling of BOP and auxiliary plant systems.

Systematic code validation is performed by GRS and independent organizations.

This manual is the first volume of the ATHLET Code Documentation comprising five volumes. The User's Manual contains the information necessary for successful code application. It presents the main features of the physical and mathematical models which the user should be familiar with in order to apply the code properly to his or her simulation task. Practical instructions and guidelines are given that enable the user to compile input data, to perform calculations, and to evaluate the results. The manual includes a complete input data description and explains the pre- and post-processing and other support software.

The ATHLET Code Documentation Package

The complete ATHLET Code Documentation consists of five volumes:

- **GRS – P – 1 / Vol. 1: User's Manual**
  The essential document for applying the code effectively. It contains the information necessary to perform successful calculations. It includes explanations, guidelines and instructions for modelling a reactor plant and running the code.
- **GRS – P – 1 / Vol. 2: Programmer's Manual**
  Companion document to the User's Manual. It contains instructions for code

installation and comprehensive lists of subroutines and variables.

- **GRS – P – 1 / Vol. 3: Validation**
  It describes the strategy and the status of code validation. It documents the validation calculations performed prior to the release of the current code version.
- **GRS – P – 1 / Vol. 4: Models and Methods**
  Comprehensive description of the basic modelling assumptions, physical models and correlations, and numerical methods in ATHLET.
- **GRS – P – 1 / Vol. 5: Program Updates**
  This document includes a listing of major program modifications.

The ATHLET Code Documentation is available to all user organizations in possession of a valid license for ATHLET.

About this Manual

The User's Manual is the most important part of the whole ATHLET Code Documentation. It contains all information that a user must know to apply ATHLET successfully.

Purpose, Scope and Structure of the Manual

A comprehensive User's Manual was written with the intention to supply in one volume all information necessary for applying a large simulation code to challenging simulation tasks.

The first concern to the user is a practical one: How to achieve results within the given limits of resources and time? Therefore, instructions are expected for compiling an input model and for running the code effectively.

The second aspect, that should be of equal concern, is the quality of the calculated results. The ATHLET code is generic in the sense that the user defines the specific simulation model by means of the input to the code. Therefore, the results reflect the combined effect of both the code and the user. It is not possible to eliminate this user effect and its contribution to the overall uncertainty altogether. However, user guidelines can keep this effect within tolerable bounds.

It is the purpose of this manual to support the user with respect to both aspects.

The scope of this manual follows the rule: Not more than necessary, but not less either. From experience with the numerous applications inside and outside GRS, we

have learned that a correct input data description with some explanatory notes is not enough by far. Users expect written instructions and guidelines. Moreover, in order to be able to perform high-quality calculations independently, the user needs background information about the underlying models and methods. It is an explicit intention of this manual to raise the user's understanding why components should be modelled in a specific way, instead of merely telling him what to do. That is why we have devoted as much space to explanations and descriptions as to instructions and guidelines.

The manual is clearly structured. The main information about ATHLET is contained in Part 1. The other four parts have specific auxiliary functions.

The structure of Part 1 is not rigid. Purposely we make no distinct separation between explanations (What is ...?) and instructions (What to do ...?). For each subject, we combine the explanation how the model works with practical instructions on its usage and special hints or warnings. Thereby, we try to avoid the inconvenience of looking for pieces of information to the same subject under different sections. Since this problem cannot be completely avoided, we include references to related chapters in the text, and we provide an Index at the end of Part 1.

For the same reason, we avoid a segregation between basic information for beginners and detailed information for advanced users. To our experience, most of the users start with rather ambitious tasks from the very beginning of their acquaintance with ATHLET, i.e. their first subject of analysis is a complicated experiment or even a reactor transient. Full information is therefore needed for all users.

Conventions used in this Manual

This manual uses several style elements like different formats, or script fonts. To emphasize terms, they can be written **bold**, underlined or in *italics*.

Equations and formulas containing general physical expressions are written in Times font in italics mode. Those of general importance are numbered to allow them to be referenced, the others with only local significance are not:

$$R_g = \frac{1}{m_g} \cdot \sum m_{gi} \cdot R_{gi}$$

Equations and formulas containing mainly ATHLET-specific expressions are written

in Courier font:

$$\mathtt{DUDT} = \frac{\mathtt{TSHN} - \mathtt{THYN} - \mathtt{TFRN}}{\frac{2\pi}{60} \cdot \mathtt{PTETA}}$$

ATHLET variable names are written in `Courier type` and always in `CAPITAL LETTERS`. This is a uniformly spaced font like computers with FORTRAN programs will produce. These variable names generally appear in the ATHLET print out or are part of the input data and you should become familiar with them. The expressions written in lower-case letters represent free (dummy) input. ATHLET input samples are written in Courier type:

```
----- pc-name
@     IPRI0    ASYSO
      -1       i
@     SBO0     ANAMO       SEO0     IARTO
      0.0      PIPE1       0.0      1
      0.0      CROSSCONN   1.0      1
      0.0      PIPE2       0.0      1
```

Also the ATHLET print output samples are written in Courier type but sometimes with a smaller font size to enable more characters to appear in one line. Again, expressions written in lowercase letters represent the actual numbers or text strings.

```
VOLUME AND MASS SUMMED UP FOR TFO NAME CATEGORIES
_____________________________________________________
 ANAMO.....   NUM.  VOLUME      TOTAL MASS
                    (M**3)      (KG)
 P.........    27   8.00501D+02 5.68129D+05
 S.........    10   7.96716D+02 1.76575D+05
 ..................................
 P0........     6   4.26941D+02 2.99845D+05
 P1........     5   1.53645D+02 1.10157D+05
 ..................................
 S1-SG.....     5   5.97537D+02 1.32431D+05
 S2-SG.....     5   1.99179D+02 4.41437D+04
 ..................................
```

A Personal Word to the User

This manual was written for you, the ATHLET user. Its only purpose is to help you to prepare, execute and evaluate the calculations for your simulation task.

Knowing the complexity of nuclear power plants and the large variety of scenarios to be simulated nowadays, we are fully aware of the challenging tasks you are confronted with. Therefore, we have given much thought to the question: What does the user really need to know, and which is the best structure for presenting the material. As you can see from the size of this manual, we think that you need to know a lot in order to fully profit from the code capabilities.

Much has been said about the *user influence* on code results, mostly criticizing that too much freedom is left to the user. The fact remains, however, that with a general and flexible code, the user must bear high responsibility for the calculated results. That's why we feel obliged to provide you with all the information necessary to meet this responsibility.

If you are a first-time user of ATHLET, you should read the manual from the beginning. The time spent there will pay off, since you can avoid problems from the start. We strongly encourage also experienced users to review the entire manual in order to enhance their knowledge. Becoming familiar with the whole volume will help you to locate specific items quickly when using it as a reference manual whenever a need arises.

We do not believe that a user's manual can answer all questions. Further supplementary information can be found in the ATHLET user area at *https://user-codes.grs.de*. The user area also offers a forum for posting questions to the developers and the community and for notifying us of any inconsistencies and problems you observe in the code behaviour.

Also, this edition of the ATHLET User's Manual may contain deficiencies and errors. Your comments and hints for improvements are highly welcome.

A successful application of large system codes cannot be learned from books alone. Training and practical experience is necessary for you to become a skilful user.

We wish you a successful work with ATHLET!

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ATHLET 3.5

User's Manual

Part 1:
ATHLET Description

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Contents

Document Updates

This document has been updated according to both the ATHLET developmental progress from ATHLET 3.4 to ATHLET 3.5 and the advanced experience of the program application. The following lists the sections modified. Please click them to follow the link!

Document updates from ATHLET 3.4 to ATHLET 3.5:

5.4	3D heat conduction in structures by coupling of HCOs
13	Simulation of severe accident related phenomena
10.17	Heat pipe module
5.7.6.2	Thermal radiation between HCOs connected to different TFOs
5.3	Simulation of horizontal plate HCO coupled orthogonally to a vertical TFO
5.6	Properties for new materials boron carbide (B_4C), Inconel 600, and Alumina (Al_2O_3)
13	ATHLET extensions to simulate severe accident related phenomena (up until start of core degradation)
10.10	Modelling of spacer grids
3.8	Positioning and 3D Data for TFO
12.3.3	TFD system monitoring under keyword `FLUIDBAL` extended. TDV mass and energy balance printed under `TDVBAL`.
10.5.2	Two-channel pressurizer model

Abbreviations and Notations

List of abbreviations:

Abbreviation	Meaning
1M	Mixture momentum equations system
2E	Two energy equations system
2M	Two momentum equations system
AFK	ATHLET function routine
ATF	Accident tolerant fuel
ATWS	Anticipated transient without scram
BOP	Balance-of-plant
BWR	Boiling water reactor
CD	Critical discharge
CDR	Critical discharge rate
CL	Collapsed level
CSA	Cross sectional area
CV	Control volume (Finite-volume-approach)
CW	Control word
DEB	Double end break
DFFB	Dispersed flow film boiling
DLL	Dynamic link library
DNB	Departure from nucleate boiling
ECC	Emergency core cooling
EIMMB	Extended integrated mass and momentum balances
Eq.	Equation
FEBE	Time integration module within ATHLET
FTRIX	Sparse matrix package within ATHLET
FV	Finite volume (numerical method)
GCR	Gas cooled reactor
GCSM	General control simulation module within ATHLET
HECU	Heat conduction module within ATHLET
HCO	Heat conduction object
HCV	Heat conduction volume (heat slab)
HTC	Heat transfer coefficient
HTEX	Heat exchanger

HW	Heavy water
IMMB	Integrated mass and momentum balances
IP	Interfacial
KW	Keyword
LM	Liquid metal
LP	Lower plenum
LW	Light water
LWR	Light water reactor
LOCA	Loss-of-coolant accident
MC	Multi-component
ML	Mixture level
NC	Non-condensable
NEUKIN	Neutron kinetics module in ATHLET
NPP	Nuclear power plant
ODE	Ordinary differential equation(s)
PBR	Pebble bed reactor
PC	Priority chain (= iteration chain)
PHX	Plate heat exchanger
PW	Pseudo-keyword
PWR	Pressurized water reactor
RBMK	Graphite-moderated boiling water reactor (Russian type)
RV	Reactor vessel
SG	Steam generator
SJP	Single junction pipe
SMR	Small Modular Reactor
SO	Shared object
SSC	Steady state calculation
TFD	Thermo-fluid dynamics
TFO	Thermo-fluid dynamic object
TRISO	Tristructural-isotropic
UH	Upper head
UP	Upper plenum
VVER	Pressurized water reactor with horizontal steam generators (Russian type)
ZB	Zinc-borate

List of notations:

Control Volume: Basic network element; spatial entity where mass and energy are lumped.

Function Routine AFK: Tree of subprograms describing the relationship between the thermal-hydraulic solution variables and the ODE system. If required, it also calls for other independent modules (HECU, GCSM, etc.).

Input Model: All input data for all modules applied in the particular simulation (including balance-of-plant models, user-supplied GCSM controllers and user-provided plugins).

Junction: Basic network element; connection between CVs where mass and energy are transported.

Simulated System: Domain of the power plant, test facility, etc., whose behaviour shall be simulated.

Simulation Model: Combination of simulation program and input model.

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 built-in 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
- plugin 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, Climate Action, Nature Conservation and Nuclear Safety (BMUKN) 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 melting 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 core melting and relocation, and debris bed formation. The simulation of the mechanical fuel behaviour as well as fission product release and transport within the reactor system is supported by both codes, ATHLET and ATHLET-CD. 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 the **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 several 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)
- Fission Product Behaviour and Transport (FPB)
- Neutron Kinetics (NEUKIN)
- Control and Balance-of-Plant (GCSM)

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 super-heated 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) plugin.

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 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.
- Optonally for coupled plate-type HCOs, the three-dimensional heat conduction can be calculated by applying dedicated solution algorithms from NuT.
- In each HCO, several 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, heat pipes, 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 weakness-es 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, . . .)
- Batchplot: Platform-independent, Python-based plotting tool that generates time

and space diagrams exploiting the structure of the input model.

- 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 AC^2 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 **AC^2 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 FEBE time step, used for coupling with CFD codes).
Moreover, ATHLET can be extended by user provided feature implementations. The **plugin 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 plugins have to be created as separate shared libraries on Linux systems or DLLs under Windows. In case a plugin 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 plugins are specified by ATHLET.

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

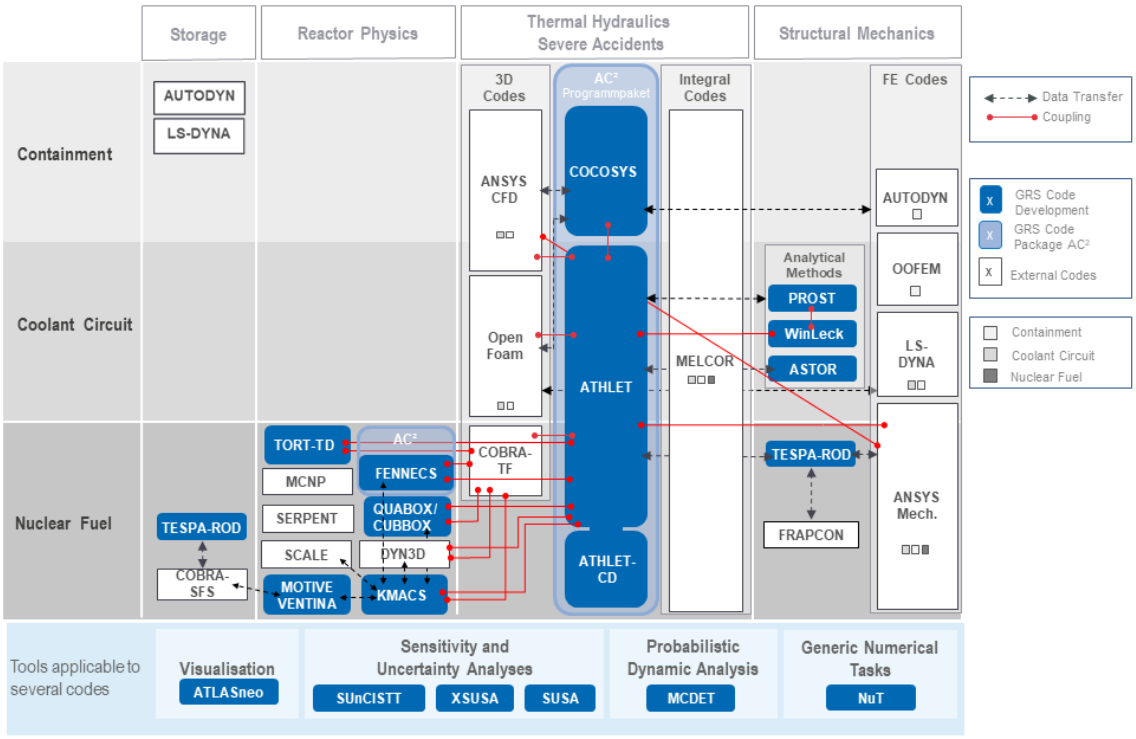

Fig. 1.1 GRS nuclear simulation chain and code coupling

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.

2 The Modular Code Structure

The ATHLET code has a modular structure. The organization of the overall code firstly corresponds to the main physical processes to be simulated:

- thermo-fluid dynamics (module TFD)
- heat conduction, heat transfer (module HECU)
- fission product behaviour and transport (module FPB)
- neutron kinetics (module NEUKIN)
- control and balance-of-plant (module GCSM)

Secondly, a modular subdivision is also applied to collect program parts which contribute to a specific task:

- time integration of the ODEs (module FEBE)
- program control and organization (module A...)

Thirdly, the code is modular with respect to program parts which are not directly involved in the ATHLET network. Since the data exchange happens only via the subprogram dummy argument list they can be easily exchanged:

- physical models
- (reactor) component simulation models

Modules can be partitioned into sub-modules. Each module and sub-module have its own leading identification (ID) letters (one for a module, two for a sub-module).

Each subprogram name starts with the identification letter of that module to which the program is assigned to. The same applies to the names of modules, where the first letter always is a 'C' and the second (and third, resp.) are the (sub-)module identification.

This allows a lexical ordering of the program parts and is very useful for the management of the source code of a large computer program like ATHLET. This classification of subprograms by letters is also helpful for better understanding of the printout, since messages and other information are often accompanied by the name of the subprogram initiating it.

The following table Tab. 2.1 contains all ATHLET code modules and their identification letters.

Tab. 2.1 ATHLET Modules

ID letter	Module	Function
A	ATHLET	control and organization module
AI		- input
AO		- output
AP		- parallel processing
C		used only for Fortran modules
D	TFD	thermal-hydraulics module
E	HEAT	adapted HEIZ module (ATHLET-CD)
EF	FIPREM	fission product release
F	FEBE	time integration module
G	GCSM	general control simulation module
H	HECU	heat conduction module
K		reactor component models
KB		- boron transport model
KC		- compressor model
KP		- pump model
KR		- heater or fuel rod model
KS		- solute transport model
KT		- turbine model
KV		- valve model
M		models
MC		- critical flow models
MD		- correlations for drift, slip, relative velocities
MF		- pressure drop (friction) correlations
MG		- interfacial mass and energy exchange models
MH		- heat transfer models
MP		- properties
M1		- CDR1D model
N	NEUKIN	neutron kinetics
NP		- point kinetics
N3		- interface to 3-dimensional kinetics
S		service programs for general use
SO		- service programs for output (print and plot)
T	SAFT	transport of fission products and aerosols (also ATHLET-CD)

TM	THEMEC	thermo-mechanical fuel rod behaviour
V		vessel failure module
VE		burn-up and radionuclide inventory calculation (VENTINA)
Z		key-file, units, interface to nuclear plant analyser ATLAS

The following table shows the naming rules for subprograms and modules. The letter 'x' represents a free alpha-numeric character.

Tab. 2.2 Naming rules for subprograms and FORTRAN modules

Assignment	**Subprogram**	**Module name**
Module	Mxxxxx	CMxxxx
Sub-module	MUxxx	CMUxxx
None of the above	-	CCxxx

18 History of ATHLET Development

Predecessor codes

When GRS was founded in 1977 by fusing the Laboratorium für Reaktorregelung und Anlagensicherheit (LRA) in Garching and the Institut für Reaktorsicherheit (IRS) in Cologne, it inherited a number of simulation codes. These were, as it was usual at the time, codes for specific reactor types and accident scenarios like ATWS or LOCA. Codes developed at LRA included the BRUCH codes /KAR 69/, /KAR 70/ from the 1960s and the DRUFAN code /WOL 75/, /BUR 79/ for blowdown analyses, ALMOD /FRI 77/, /FRI 78/ and ALMOS /PET 75/, /PET 77/ for transient analyses, DAPSY for pressure wave analyses /GRI 83/ and neutronics codes like QUABOX/CUBBOX /LAN 78/, which would later influence ATHLET development.

Already in 1975, DRUFAN participated in the USAEC Standard Problem 1 and achieved reasonable results /WOL 75/ with a focus on blowdown scenarios /WOL 76/. Its further development for two-phase flow problems was achieved within GRS. DRUFAN 01 in 1979 was based on a 4-equation model allowing thermal non-equilibrium conditions /BUR 79/, /GRS 79/ and used some constitutive models from e.g. the BRUCH codes. The HECU code /DAS 76/ was already integrated /ENI 78/, as was a point kinetics model from ALMOS-2.

DRUFAN 02 included numerous model improvements, a relative velocity model, a mixture level tracking model for vertical geometries and allowed for mechanical non-equilibrium conditions, included improved control module, critical discharge models, and separator models /LER 85/. The code assessment of DRUFAN was based on tests like Battelle RS Tests and HDR tests, mainly blow-down tests, and integral tests at LOFT, LOBI, SEMISCALE, and PKL.

In parallel, ALMOD /GRA 86/ and its BWR variant ALMOS had also been further improved. While still assuming a 3-equation homogenized equilibrium model with a drift-flux approach for fluid dynamics, the code included the GCSM module used for both I&C representation and for simplified system models and the NEUKIN module with point kinetics and 1D kinetics options. In addition, the IMMB approach (integrated mass and momentum balances) was available to reduce computational costs. ALMOD had been validated against separate effect tests, LOFT and LOBI tests as well as several plant transients in German NPP /FRI 85/.

In addition, development of the FLUT code using a two-fluid 6-equation model /HIC 85/ for analyses of the refilling and long-term phases after the blowdown phase was

progressing well. Notably, FLUT already included a quenching model as well as a water level tracking model, and had been successfully validated against FEBA, FLECHT, PKL and SCTF tests. Moreover, a transition procedure from DRUFAN to FLUT was established.

With the development of multiple codes ongoing at GRS and with several tasks for the implementation of models and codes performed by specialists in the IT division of GRS, a systematic and quality assured development process was necessary. Therefore, roles for developers and code maintainers were clearly defined, version control was implemented by clear procedures for the modification of the code and transfer into the main development and release branches. Logs for code changes were accompanied by internal communications and technical notes for documenting development, verification and validation activities. Moreover, regular meetings of development teams ensured communication between the main developers and validation specialists.

ALMOD/ALMOS and DRUFAN had been distributed by GRS to numerous partners, notably the German TÜV and several national and international research organizations. DRUFAN was also available via the OECD/NEA code data bank.

Recognizing the need for one system code for these different application areas, GRS decided in 1984 to combine its extant system codes into one advanced system code. With concepts and a code specification drawn up by mid-1985 /WOL 85/, the codes DRUFAN, ALMOD and FLUT were combined into the new, yet unnamed system code, with a first internal version available in 1986 /WOL 86b/ and the final name established towards the end of 1986 /WOL 86a/. The first validation calculation with ATHLET published as a project report was on the Marviken test in 1987 /RIN 87/.

First ATHLET version

The first ATHLET version, ATHLET MOD1, was released in 1988 /GRS 88/, /BUR 89/. Overall, ATHLET was based on DRUFAN using the non-equilibrium fluid dynamics and mixture level tracking and the common HECU and FEBE modules while fully importing the GCSM and NEUKIN models from ALMOD/ALMOS. Simplified fluiddynamic models from ALMOD were initially retained. ATHLET used FORTRAN 77 and was implemented on mainframes as well as PC computers. In the meantime, FLUT development was continuing and the existing coupling of DRUFAN to FLUT was transferred to ATHLET. In conjunction with the release of ATHLET MOD1, further substantial validation and verification was initiated by GRS, which also involved

external organizations from German TSOs (TÜVe) and research institutions, e.g. Ruhr-Universität Bochum (RUB). This effort did not only include a substantial amount of validation cases from the recently defined validation matrices /NEA 87/, it did also include an external review of the models and coding of certain ATHLET modules, e.g. GCSM /BAU 93/ and HECU /LIN 93/. Highlights of the further development of ATHLET are depicted in Fig. 18.1.

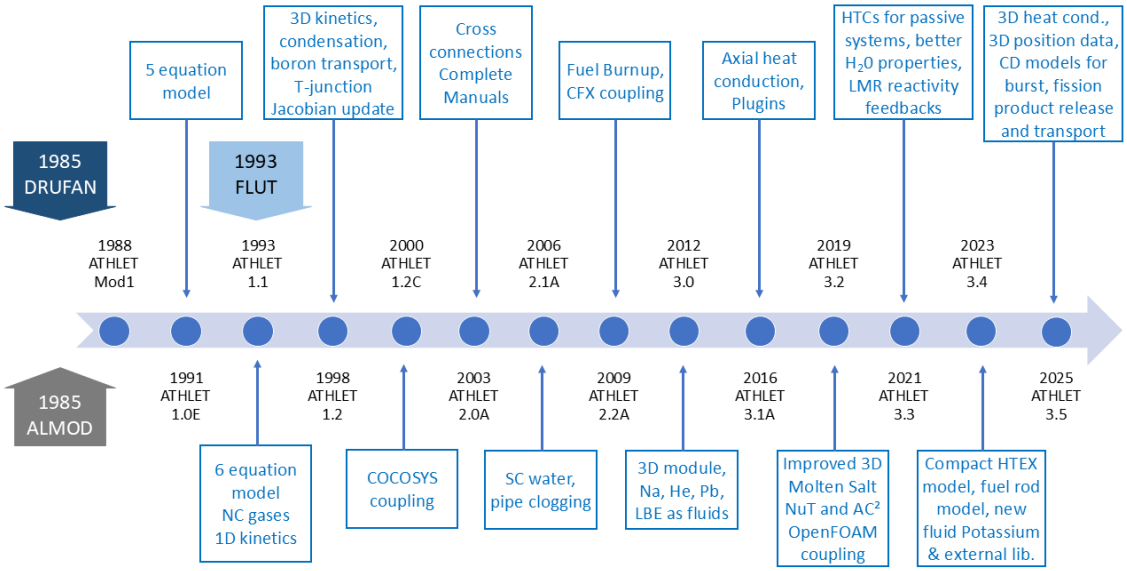

Fig. 18.1 Timeline of ATHLET development

The initial development progress was quite high. ATHLET version 1.0E introduced a 5-equation model with separate energy balance equations for gas and liquid phase in 1991 /BAL 91/. Further improvements included introduction of cross-connection objects, improvements in the separator model and a Zr oxidation model /TES 96/. ATHLET 1.1 from June 1993 included improvements to the 5-equation model, replacing the 4-equation model as standard option, improvements to mixture level and interfacial models, a quench front model and the coupling to the containment code CONDRU via GCSM. CONDRU /TIL 78/ was one of the containment codes developed by GRS before COCOSYS and had also been validated against e.g. OECD NEA standard problems /TIL 79/, /ERD 81/. Into this version also a first 6-equation model adapted from the FLUT code based on a two-fluid model with separated balance equations for the two phases and considering thermal and mechanical non-equilibrium conditions to calculate the mass, momentum and energy exchange between water and steam was implemented and made available internally at GRS. This model was further elaborated and complemented with improved interfacial friction and condensation

models and extended to non-condensable gases /TES 96/. Similarly, radiation heat transfer and boron transport were added /PET 94/. A large factor in improving numerical stability was increased control over the Jacobian matrix and its updates.

Another important strain for the development and validation of ATHLET was the scientific cooperation with Eastern European countries operating VVER and RBMK reactor designs, which had started already in 1987 with intergovernmental agreements with the Soviet Union and also Eastern Germany. These activities led to the development of nodalization schemes for VVER /TES 92/, /STE 93/ and RBMK /LAN 93/, extended the validation base of ATHLET by experiments e.g. at the ISB, KSB and PMK facilities as well as plant transients and motivated the inclusion of specific models like the graphite reflector feedback, specific CHF-correlations for RBMK and VVER, and improved correlations for horizontal steam generators. Cooperation with partners in Belarus, Bulgaria, Czech Republic, Hungary, Lithuania and Slovakia further extended the user group and specific validation activities.

The possibility to simulate a complete LOCA process within ATHLET led to increased international interest in the code, with over 20 external users in Germany and nearly 30 users abroad, mainly in Europe and Asia. Version ATHLET 1.1C was released in October 1995 /TES 97/. In order to simplify the modelling of non-condensable gases, phase enthalpies were replaced by temperatures as solution variables. In addition to a boron transport model, a 3D neutronics interface and component models for T-junctions and pressurizers, several code and tool optimizations were realized. ATHLET 1.2 was released in 1998 /TES 97/, /TES 01/ providing the 6-equation model also for external users. In addition, it included further improvements like improved models for interfacial processes in the presence of non-condensable gases, computation of heat transfer in the fuel gap, specific heat transfer correlations for horizontal heat exchangers of VVER reactors, and improved integration routines with partial Jacobian updates. Notably, this was the first release version for PCs, so that ATHLET was now being developed for both Windows and Unix/Linux systems. The code version 1.2C from November 2000 included a first implementation of coupling between ATHLET and COCOSYS. Moreover, a jet condensation model, better interfacial friction models, CHF correlations for RMBK and research reactors, gas mixture transport properties and improved mass conservation had been realized. In addition, the source code had been transferred to the Fortran 90 standard with free format input. In particular, the modules for ATHLET global variables were introduced and allocatable arrays were introduced /DEI 99/, removing most hard-coded restrictions on problem size.

ATHLET version 2

In 2003, ATHLET 2.0A was released. It included further improvements to the models for condensation, mass and energy transfer at the phase interface, transport of dissolved nitrogen, and introduced parameters. Improved cross-connection object flexibility enabled the simulation of cross flows to better represent multidimensional flow behaviour in large components such as the RPV. Also, this was the first version accompanied by the complete code documentation: a user's manual, a programmer's manual, one volume on validation and one on the applied models and methods /TRA 04/. With this version, a first GUI for Windows, tools like ATHLET input graphics and GCSM input graphics and the interactive simulator interface ATLAS were distributed. Since then, ATHLET and ATHLET-CD were released jointly with the same version number.

ATHLET 2.1A from 2006 extended the parameter range for water to supercritical pressures, including the calculation of material properties and heat transfer correlations. In addition to numerous general improvements to different models, this version automatically switched to the 3-equation model for single-phase flow, integrated the CRD1D model for critical flow calculation, added a Zr oxidation model in the presence of oxygen, provided an interface of uncertainty analyses /TRA 09/ and introduced a model to simulate the clogging of pipes /LER 06/. The models for supercritical fluid including specific heat transfer correlations and sump strainer clogging were further improved in ATHLET 2.2A /GLA 12/, /LER 09/ released in 2009. This version also included a model for diffusion of gas components, allowed consideration of fuel burnup for neutron kinetics, introduced additional material properties for UO_2 and MOX, and allowed binary operations with parameters. Importantly, this was the first ATHLET version allowing partial parallelization, it established the coupling to the CFD code ANSYS CFX®. The following release was ATHLET 2.2B /GLA 12/ in 2011, which included heavy water as a working fluid (derived from light water properties), improved steady state calculation, consideration of burn-up in fuel thermal conductivity, and further improvement in specific models. In addition, the input deck could use includes and pipes connected at their ends in priority chains were automatically coupled.

ATHLET version 3

The next major release was ATHLET 3.0A in 2012, which introduced the new working fluids heavy water, liquid lead, sodium, helium and lead bismuth eutectic. This version also added the option to utilize 2D or 3D momentum equations as well as the possibility to simulate pebble bed reactors. Additionally, new models for spray

condensation and turbines were implemented /GLA 12/, /LER 12/. With this version, ATHLET was maintained in a subversion repository, so that all commits to the current master version are fully traceable. ATHLET 3.1A from 2016 implemented a model for axial heat transfer in heat conduction objects, improved the 3D momentum models and added an option to use cylindrical coordinates. Turbine models were further improved, and argon was added as a new non-condensable gas. This version also introduced the plugin technique to allow for easier coupling with external modules /SCH 15/, /LER 16/. More than 50 organizations held a license for ATHLET 3.1A.

Since 2016 much effort was spent on improved code coupling and the plugin concept was further enhanced and several new plugin interfaces were made available in ATHLET, enabling the user to extend ATHLET capabilities by using their own models or correlations, e.g. for material properties, heat transfer or critical heat flux calculation /LER 19/. Further improvements were implemented with a view to advanced Gen-III/III+ LWRs, SMRs and also Gen-IV reactor designs with a specific focus on passive safety systems /SCH 18/. These developments are included in ATHLET version 3.2, which was released in June 2019 as part of the software package AC^2 2019. It also introduced supercritical CO_2 and molten salts as working fluids and offered the Numerical Toolkit (NuT), which allows access to alternative numerical solvers to speed up calculations.

In the year 2021, ATHLET 3.3 was released. It came with an optional new water property package developed by HSZG, geometric reactivity feedback for liquid metal reactors, additional heat transfer correlations for passive systems, new non-condensable gases, as well as multiple code improvements.

ATHLET 3.4 was released in 2023. ATHLET 3.4 comprises an extended fuel rod and gap conductivity model, that is capable to consider fuel swelling, densification, and radial relocation. In addition, dedicated heat transfer coefficient and friction factor correlations for compact heat exchangers such as plate heat exchangers are included, which allow an improved simulation of e.g. SMR reactor designs. Potassium is introduced as new two-phase working fluid. Further working fluids are available through the property package library CoolProp, which can be coupled to ATHLET. Krypton and xenon are offered as further non-condensable gas components.

The current version ATHLET 3.5 was released in 2025. It allows more than three material zones in HECU objects and heat conduction between HCOs and it includes a dedicated heat pipe module. Moreover, flow regimes are now calculated centrally and consistently for all models. Additionally, 3D position data can be specified for

TFO and 3D data in a vtm format can be obtained for TFO and HCO. Furthermore, ATHLET 3.5 includes the first results of the integration of ATHLET-CD models: a blockage model for fuel rods up to cladding burst, radiation heat transfer between HCOs, and fission product transport is available via the SAFT module. Moreover, VENTINA can be used to define radionuclide inventories and compute their decay in an initial version.

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