ATHLET
Mod 3.0 Cycle A

Program Overview

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1  Overview of ATHLET

The thermal-hydraulic computer code **ATHLET** (Analysis of THermal-hydraulics of LEaks and Transients) is being developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (**GRS**) for the analysis of anticipated and abnormal plant transients and all kinds of leaks and breaks first and foremost in light water reactors. Moreover, the code can also be applied for plants and facilities applying the working fluids heavy water, helium, sodium, lead or lead-bismuth eutectic.

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 and BWRs with only one code. The main code features are:

- advanced thermal-hydraulics
- modular code architecture
- separation between physical models and numerical methods
- pre- and post-processing tools
- portability

ATHLET is being applied by numerous institutions in Germany and abroad.

The development and validation of ATHLET is sponsored by the German Federal Ministry of Economics and Technology (**BMWi**).

1.1  Range of Applicability

ATHLET has been developed and validated to be applied for all types of design base and beyond design base incidents and accidents without core damage in light water reactors, like PWR, BWR, VVER, and RBMK. For accidents with core damage, ATHLET-CD has been developed providing extensions for the simulation of the mechanical fuel behavior, core melting and relocation, debris bed formation as well as fission product release and transport.
The range of applicability has been extended to supercritical water enabling the transition from super- to subcritical fluid states. In addition to light water, further coolants can be simulated as working fluids: heavy water, helium, liquid sodium, lead and lead-bismuth eutectic. These extensions are still subject of further development and validation.

1.2 Code Structure

The ATHLET structure is highly modular so it allows an easy implementation of different physical models. The code is composed of several basic modules for the calculation of the different phenomena involved in the operation of a light water reactor:

- Thermo-fluiddynamics (TFD)
- Heat Transfer and Heat Conduction (HECU)
- Neutron Kinetics (NEUKIN)
- General Control Simulation Module (GCSM)

The 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 a general interface.

ATHLET provides a modular network approach for the representation of a thermal-hydraulic system. A given system configuration can be simulated just by connecting basic fluiddynamic elements, called thermo-fluiddynamic objects (TFOs). There are several TFO types, each of them applying for a certain fluiddynamic model. All object types are classified into three basic categories:

- **Pipe objects**: apply for a one-dimensional TFD-Model with partial differential equations describing the transport of fluid. The nodalization (number of nodes or volumes) is defined by input data. After nodalization, a pipe-object can be taken as a number of consecutive volumes (control volumes) connected by flow paths (junctions). The mass flow rates at the volume boundaries are calculated by the solution of momentum differential equations (local momentum balance) or by algebraic equations when the integrated momentum balance option is chosen. The calculation of the mass flows at the inlet and at the outlet of a pipe object is included in the pipe object model. A special application of a pipe object, called single junction pipe, consists of only one junction, without any control volumes.

- **Branch objects**: apply for any TFD-Model described by an arbitrary system of non-linear ordinary differential equations or even algebraic equations.
• **Special objects:** used for components with complex geometry (e.g. the cross connection of pipes within a multi-channel representation).

Each fluiddynamic object provides a subset of the entire ordinary differential equation (ODE) system of the fluiddynamics, which is integrated simultaneously (time advancement) by the ODE-solver FEBE. Within the pipe objects, the ODEs are obtained from the partial differential equations by applying a spatial approximation method.

This object structure has been developed in order to allow the coupling of models of different physical formulation and spatial discretization techniques. The inclusion of new models (e.g. new object types) is facilitated by a standard implementation procedure, independently of the physical assumptions contained in the model.

## 1.3 Fluiddynamics

ATHLET offers the possibility of choosing between different models for the simulation of fluiddynamics:

- **5-equation model,** with separate conservation equations for liquid and vapor mass and energy, and a mixture momentum equation. It accounts for thermal and mechanical nonequilibrium and includes a mixture level tracking capability,

- **Two-fluid model,** with separate 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 approach. The mass and energy equations are solved within control volumes, and the momentum equations are solved over flow paths (junctions) connecting the centers 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 countercurrent flow limitations in different geometries.

Moreover, both fluid-dynamic options allow for the simulation of non-condensable gases on the basis of the ideal gas formulation. This applies also for the liquid metal working fluids. Additional mass conservation equations can be included for the description of boron transport within a coolant system as well of the transport and release of nitrogen dissolved in the liquid phase of the coolant.

For pipe objects applying the 5-equation model, there is also the possibility to use the method of integrated mass and momentum balances (EIMMB - Method), an option for fast-running calculations, mainly in the frame of a nuclear plant analyzer. 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.

So far, the one-dimensional conservation equations for mass, momentum and energy are implemented in ATHLET. Certainly, by means of spatially two- or three-dimensionally arranged TFOs, these equations admit of simplified multidimensional simulations even now. In order to enhance the capabilities of ATHLET in simulating complex, multidimensional flow phenomena, an additional 2D/3D module is currently under development. At this stage, the fully two-dimensional momentum equations for liquid and vapor are available. However, since developmental and validation work are still in progress, their application is only recommended for test and research purposes.

### 1.4 Numerical Methods

The time integration of the thermo-fluidodynamics is performed with the general purpose ODE-solver called **FEBE** (Forward-Euler, Backward-Euler). It provides the solution of a general non-
linear system of differential equations 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.

The linearization of the implicit system is done numerically by calculation of the Jacobian matrix. A block sparse matrix package (FTRIX) 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.

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 determined for every integration step.

### 1.5 Heat Conduction and Heat Transfer

The simulation of the heat conduction in structures, fuel rods, and electrical heaters is performed within the basic module **HECU**. It permits the user to assign heat conduction objects (HCOs) to all thermal-fluiddynamic 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 geometry 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.
- In each HCO, up to three material zones can be modelled. A material zone is simulated by a problem dependent 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 decompose automatically 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.

The heat transfer package covers a wide range of single phase and two-phase flow conditions. 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 as well for specific geometries (e.g. 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 be optionally 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 behavior of the prompt power generation is calculated either by a point-kinetics model or by an one-dimensional neutron dynamics model. 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 prompt 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 **one-dimensional model** solves the time-dependent neutron diffusion equations with two energy groups of prompt neutrons and six groups of delayed neutrons. The active core zone can be subdivided into zones with different materials. A reflector zone is also considered.
The model includes the coarse-mesh spatial approximation of the neutron flux by means of second order polynomials. It also accounts for moderator and Doppler reactivity feedback by temperature and density dependent cross sections. Control rod movement and reactor scram are simulated by means of local changes of group cross sections as a function of rod position. Libraries of effective cross sections for several types of light water reactors are also available.

The module NEUKIN offers also 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.

### 1.7 Simulation of Components

In general, major plant components (e.g. pressurizer, steam generators) can be modelled by connecting thermo-fluidynamic objects (TFOs) and heat conduction objects (HCOs) via input data. Simplified compact models for those components are also available as special objects.

Additional models are provided for the simulation of valves, pumps, accumulators, steam separators, steam and gas turbines, steam condensers, single and double ended breaks, fills, leaks, and boundary conditions for pressure and enthalpy. Except for the separator model, they are comparable to the corresponding models in other advanced codes. 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.

Critical discharge flow is calculated by an one-dimensional thermodynamic non-equilibrium model with consideration of the current geometry of the discharge flow path. A module, called CDR1D, generates automatically the input tables needed in ATHLET for 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-plants (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 fluiddynamics, neutron kinetics or within other ATHLET modules (process variables) can be selected as input to these functional blocks. The output of such control blocks can be fed back to the thermo-fluiddynamics in form of hardware actions (e.g. valve cross sectional area, control rod position) or boundary conditions (e.g. temperature, heat and mass sources).

This simulation module allows for the representation of fluidynamic systems (e.g. steam line, condensate system) in a very simplified way (quasi stationary approach) with the advantage of requiring very little computation time in comparison with the fluiddynamics module.

GCSM also provides a general interface to an external library of BOP models. This library contains detailed models with fixed structure and own input data for plant components (e.g. turbine, or even a containment model) or for control systems (e.g. power control, feedwater 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.

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. An extended checking of both the input data and the program processing helps the user to discover input errors or modelling weaknesses affecting the code performance.

ATHLET provides a restart capability. The program execution can be parallelized on computers with shared memory architecture using the Fortran OpenMP standard.

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:

- G2: Generates GCSM input data from control diagrams (proprietary, license required).
- AIG: Graphical representation of the thermo-fluid and heat conduction objects of the input model.
- GIG: Graphical representation of the structure of GCSM controllers.
- Several programs for the post-processing of plot data (concatenation, merging, algebraic operations,...)
• JSPLOT: Generates time and locus diagrams exploiting the structure of the input model.

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• ATLAS-DyVis: 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,..)

Furthermore, ATHLET can be applied as process model of the ATLAS plant simulator providing full interaction and extended data visualization.

ATHLET runs under different computer operational systems (Windows, Unix, Linux,...). All supporting programs run under Windows, some of them also under Unix / Linux.

1.10 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 real 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 in all common LWRs. The validation of ATHLET in the field of advanced reactor designs (Gen IV) is underway.