Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

ATHLET 3.2

Program Updates Since
Release ATHLET 3.1A

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Program Updates and Patches Since Release of Version 3.1A; Known Program Errors

This document lists the major program modifications of the current ATHLET version since the last general release version 3.1A. It provides information not only for the ATHLET users but also for the developers, i.e. it may contain details which are not relevant for normal code users.

Further information on program modifications relevant for ATHLET applications can be found under Document Updates of the *User's Manual* as well as under Input Data Updates of the *Input Data Description*.

On ATHLET patches: Although ATHLET is comprehensively tested and validated before it is released, program errors or shortcomings cannot be completely avoided. There are several reasons for that:

- The test cases we use don't cover the whole range of applicability of ATHLET.
- We cannot foresee all the possible errors that could occur when the program is applied.
- Novel applications may require new models, changes in proper use of models, or adjusted or extended input and run time checks.
- User feedback may indicate needs of program modifications.
- Despite our best efforts, a code with scope and complexity as ATHLET will never be free of weaknesses or errors.

Released ATHLET versions are patched whenever it is necessary or appropriate. Patches are classified as

- **Critical**: Program errors are fixed which could significantly impair the quality of results or reliability of code application. In that case, all users will be informed via ATHLET User Area. The user is strongly recommended to update his ATHLET version.
- **Non-critical**: The code performance, reliability and/or user convenience are improved. Particular applications may require program updates which are not needed for usual applications.

Important known issues with the code and their resolution or applicable work-arounds are documented in the ATHLET User's Area on the GRS website and summarized in section 2 of this document.

1 Program Updates in ATHLET 3.2

Bold face indicates that user's action may be required even for existing input decks.

1.1 Thermo-Fluiddynamics

- Evaporation and condensation (hence two-phase state) of working fluid sodium enabled.
- **New correlations for approximation of LM properties implemented. This requires enthalpy values for fills and TDVs different to those of A3.1A (s. M&M)!**
  Recommendation: Calculate the enthalpy from p and T using the GCSM controller PROP.
- New working fluids:
  - Supercritical carbon dioxide
  - Molten salts FLINAK, FLIBE
  - User-provided simple (non-boiling) working fluids
- 3D-model extended by ML capability
- Junctions branching off from a ML track may now be vertical, too.
- **Explicit drift flux model is no longer applicable.**
- New model for condensation-induced water hammer.
- **CW `BORTRANS`: name of tracked solute has to be input, `IBDEB`<0 no longer valid;**
  own table of maximum solubility may be provided.
- **CW `OBJECT`: PW `EVAPORATE` no longer valid;**
- **CW `MISCELLAN`: `AA` must be 0.0!**
- New options to reduce / mitigate pressure wave propagation during zero-transient calculation (s. Input Data Description; CW ZEROTRANS).

1.2 HECU

- Modification of DNB calculation: DNB only dependent on CHF and no longer on minimum film boiling temperature. Min. film boiling temperature still used for onset of stable film boiling (end of transition)
- Radiation model extended: Simple treatment of radiative heat exchange between HCO surfaces and the environment realized. As a side effect, a new keyword TFO has to be input for the application of the already existing TFO-related radiation model in order to distinguish between both models (radiation to the environment and TFO-related radiation).
- MASL calculation:
  - MASL calculation starts from beginning of transient calculation.
  - `ASL0` and `THM0` used in SCAT method are now calculated by ATHLET
    (Input data `ASL0` and `THM0` are only used as starting values for stationary iterations.)
  - MASL calculation is stopped if core mass flow approaches zero.
- Heat exchanger model: New option `IQHTX=2` for adaptation of heat transfer profile only
- Quench front model applicable for pressure < 50 bar (formerly: 30 bar).
- Calculation of fuel pellet center temperature modified (extrapolation from inner layer to center of cylinder).
- Print / plot output extended:
  `HCORS`: total enthalpy stored in materials of any type of rod (reference temp. = 20 °C)
  `ISURFM`: HCV index where max. surface temperature occurs
  Single and total rod surface area (print)
  Single and total heat exchanger surface area (print)
  Heat flux in `RODLEVEL` and `CORESUM` (plot and print): `QACOR`, `QACORS`, `QACORM`
  Linear heat generation rate `LHGR` per rod in W/cm (plot and print)

1.3 Neutron Kinetics

- 3D neutron kinetic codes coupled as plug-in (QUABOX/CUBBOX, DYN3D, PARCS)

1.4 Numerical Solver

- Monitoring of increments of solution variables extended (s. CW INTEGRAT, PW DEBUG)
- Numerical Toolkit (NuT) plugin enables usage of scalable solver packages PETSc or MUMPS (see separate documentation)

1.5 Component Models

- New heat exchanger option for SSC: IQHTX=2 iterates HTEX power profile but doesn't adapt HTEX surface
- CDR1D tables are tagged in input file. New generation of tables is automatically triggered when required.
- CONDRU is now available as plugin (no longer implemented in ATHLET).

1.6 GCSM

- **As GCSM block name (BLNAME), following expressions are no longer valid**:
  AIDA, BLOCK1, COCOSYS, COMPARATOR, CONDRU, CORESUM, COUNTER, DECAY, DT2, GENERAL, HEATHEX, INTEGRAL, LEVEL, MASSLOSS, MONITOR, PIPE, PI_REGLER, SETPOINT, TFDGENERAL
- Deprecated models removed from GCSM library (boron tracking, homogeneous volume, accumulator model, containment model, SG level control)
- New process signals TSURFMAX, RELOMET, RELOCER, LPDISMASS and LHGR available.
- Process signals may be directly derived from 'visible' global variables, which are provided for every CV or HCV.
- Print/plot output
  - of GCSM signals can be controlled (CW OBJECTCON, PW GCSM)
  - GCSM hardware actions are compiled under block name HW-ACTION

1.7 Plug-ins

- **All plug-ins must be activated under CW PLUGIN.**
- New plug-in for XL correlations (MASL method).
- New plug-in for CHF correlations.
- New plug-in for user-provided simple (non-boiling) working fluids.
- BOP model has to be provided as plug-in (example available)
- Watchdog plug-in to trace the stability of an ATHLET run and terminate the simulation in case that predefined critical conditions are hit.

1.8 General

- **Modified ATHLET start parameters**: two parameters are mandatory: input file name and run identifier. Problem-ID, -rd, -r etc. deprecated. (see User Manual)
- CW `TOPOLOGY`: Input value `ISYS0` (index of fluiddynamic system – integer) changed to `ASYS0` (name of fluiddynamic system – string). The same holds for `AMCSYS` (former `IMCSYS`) under CW `MULTICOMP`.
- New sample case “VVER-1000” (generic)
- A line of the input file may consist of up to 720 characters
- ATHLET code structure:
  - ATHLET *exe*-file is mini executable that invokes the ATHLET shared library.
  - Core-degradation (ATHLET-CD) is now a plug-in invoked by ATHLET (if required)
- Generation of HTML-output requires start parameter -html (`HTML ON/OFF` in input file deprecated). HTML-output format revised.
- Command `PRINT ON/OFF` (first row of input deck) is now start parameter: -printon
- New output file **.log*: contains major information of simulation run and input listing

- Number of new hooks for ATHLET simulation control by external program (see Programmer's Manual)
- Changeover from Fortran-77 to Fortran-90 (**.f90*)
- Max. number of generated restart data sets via ISREST, EXT coupling and signal handler: 10000. Beware of .re file size!
- CW `REDEFINE`: Some quantities may be redefined for all junctions (and not only for a single junctions) of a TFO.
- Several error messages improved.
- New Intel and GNU compilers applied: Release version generated with Intel 16.4.
- **Input and run time checks extended, e.g.:**
  - `IPRI0/=1` no longer valid for PCs containing CVs. The steady state pressure distribution in the simulation system is not a free input data; must be calculated by SSC!
  - Heights of TFO and related HCO are checked for consistency.

1.9 GUI / Tools

- Optionally, plot data may be generated in Hdf-5 format (instead or in addition to pd-format). Requires activation of Hdf-5 plug-in.
- New, platform independent GUI to start AC² calculations (including couplings and NUT). As an interim approach, the former ATHLET GUI is still applicable to run ATHLET utilities.
- ATHLET Input Graphic extensively revised (AIG-2)

2 Known Program Errors

The table below lists major known bugs and shortcomings that are existent in the current program version. In addition, the program version where the respective error was detected first is given. However, the particular error may already be existent (but not found) in earlier code versions as well.

Table 1: Known Bugs in ATHLET version 3.2

Bug Description	**Existent since code version**
HCO Geometry: Assignment of HCV to wrong CV of coupled TFO Error may occur for non-parallel HCO and TFO (e.g. in heat exchangers). Possible workaround is partition of TFO into several objects each coupled to the HCO along the appropriate length. Measure in code: Extended input checks to detect assignment error and inform user	3.1A and former versions
Supercritical CO^2 property package: Properties are available in the range 73.773 bar < p < 300 bar and 283 K < T < 675 K. Accuracy deteriorates in the neighborhood of the critical point, therefore it is not recommended to use the data below 90 bars and 42 °C (315 K). Measures: The mass balance should be checked carefully.	3.2
Program abortion due to low pressure It was found, that ATHLET sometimes stops because pressure falls below lower limit of water-steam property package. The problem occurred in CV with significantly subcooled liquid, e.g. in the ECC injection pipe, and during phases with pressure disturbances, e.g. connected to high condensation rates somewhere inside the coolant system. Reasons may be too small/late evaporation (at low vapor saturation pressure) or uncertainties in the material properties at low pressures. The problem is under investigation. Measures: Modify nodalization of the region where the problem occurs.	3.1A
Form losses and turbulence model in 3D model: Optionally, viscous shear stresses and turbulent friction can be considered in	3.1A

momentum equation of 3D model by activating an in-built zero-equation turbulence model (only reasonable for highly resolving meshes). Consequently, for wall-distant junctions the standard wall friction is no longer employed. In addition, form losses are also not calculated. This may be not desired or even erroneous in the case of small scale internals (not resolved by the numerical grid) and form losses automatically introduced by ATHLET to compensate for pressure recovery due to increasing flow area along a junction. Measures: None. Use 3D model without turbulence model (recommended approach for grids with large scale CV).	

3 Patches since First Release 3.1A

The following lists the ATHLET program patches since the release of ATHLET 3.1A.

Bold face shows the chief cause of releasing a new ATHLET patch (if there is one). Others are program improvements provided on occasion of patching ATHLET to improve overall code performance for both users and developers.

03.05.18 ATHLET 3.1A Patch #04 released

01.05.18 New GCSM process signal type PSTAGE: provides power generated in the selected stage of the turbine set in [W].

Example: SPV0=5. would be stage 5 of the turbine set related to OBJNAM.

25.03.18 Auto activation for plug-ins. If a compatible plug-in is present in bin/plugin, its procedures initialize_c and execute_c will be automatically called by ATHLET.

08.03.18 Improved error bounds for ML mass fraction as well as demand of additional Jacobian updates after ML transfer reduce unreasonable high mass error which may occur in cases of very fast ML movement.
=> Restart files of former ATHLET runs are no longer applicable!

07.03.18 New Hooks available, please see Programmer's Manual, chapter 4.3

05.03.18 Libadt update. Please use `connectCallback` instead of `setCallback` if you are using hooks with a FORTRAN code. Python is not concerned thanks to an alias.

08.02.18 New GCSM process signal type LPDISMASS available (total mass discharged from lower plenum; module AIDA)

29.01.18 ML transition: If iteration of ML quantities did not converge for a falling ML, XQMO (above ML) is set to former value (may improve stability).

IGAM0 controls now the reduction of mass exchange rates at low void fraction, too. Up to now, this was always active. Hence, reduction can now be switched off.

GCSM: All hardware actions are now available in the plotting data under Block Name HW_ACTION.

New input data checks added.

18.12.17 New GCSM process signal type RODSEGPOW: provides power generated in one single HCV of a rod component.

08.11.17 Modification of multiplication factors for uncertainty analyses OFI2H, OFI2V. The two phase flow multipliers were corrected. Currently, they are void fraction dependent. For single phase water flow, the factors written in input are transformed to value 1.

13.10.17 Edit input-reading procedure to pass any extra argument through a new scope. In order to get a non-ATHLET argument and its value, please use:

```
arg_scope => getScope( root_scope, 'global', 'arglist' )
!get input parameter argname (in this case, a string)
parameter_input = char(string(get(arg_scope, '-argname')))
```

11.10.17 Libadt has been updated from 2.5 to 2.6 without any effect on calculation results. Please change the properties for the linker, if you are building your own plugin.

22.08.17 Correction for direct heating using coupled simulation with 3d-kinetics

18.07.17 ATHLET 3.1A Patch #03 released

Non-critical patch, however module CONDRU was not correctly compiled in Patch #02 for Linux application

05.07.17 1M model: Limitation of |relative velocity| to < 100 m/s
Reason: Relative velocity can increase very fast while the limitation through entrainment is damped via time lag; this may lead to numerical problems.

29.06.17 Module CONDRU compiled and linked with correct compiler option "save all variables"

28.06.17 New process signals TSURFMAX, RELOMET and RELOCER available

TSURFMAX:	Max. surface temperature in core
RELOMET:	Relocated metallic mass (ECORE module)
RELOCER:	Relocated ceramic mass (ECORE module)

22.06.17 New control of print/plot output of GCSM signals:

Needs additional input data under CW OBJECTCON after PW HCO:

GCSM Signal Control Data (PW GCSM)

This PW is only to be input if the general control data shall be overwritten for the GCSM signals.

Input:

IOUTG0

If desired:

YNAME IOUTG

: :

Explanation:

IOUTG0: Controls output of GCSM signal values:

=0: No signal is output (except problem time signal)

=1: All signals are output

YNAME: GCSM signal name

IOUTG: Controls output of signal YNAME (s. IOUTG0)

31.05.17 ATHLET 3.1A Patch #02 released

Non-critical patch

12.05.17 Correction of restart structure for scoop in combination with gas-release.
Restart-Files are no longer compatible with patch#01.

20.03.17 Binaries are now tagged with SVN-version and compiler information

08.03.17 New check of validity of `CDR1DIN` input data

06.03.17 Callback hook IDs modified (see Programmer's Manual)

06.03.17 Additional retrace trigger via visible scope-variable *retrace_request_idx* in module CAOR (dll-Version only)

16.02.17 Balance of Plant (BOP) models can be used as plugin

14.02.17 'Explicit' drift model (`JDRIFT>10`) is no longer valid; -> program stop

Lengths of input character strings must be <= 10; -> program stop

Specific heat of graphite: error for T > 1500 K fixed

17.01.17 New WATCHDOG plugin to "early-terminate" ATHLET if one or multiple critical conditions are attained. These conditions can be formulated as GCSM signals. Based on the employed watchdog function, the supervision can be permanent or temporarily enabled during the computed time.

13.12.16 MASL calculation is stopped if core mass flow approaches zero.

CDR1D table in input deck is tagged now with date of generation and used ATHLET program version; new tables will be generated when Patch#02 is applied first.

17.11.16 Start of a ML in CVs with (pure) NC gas improved

Condensation at ML surface in presence of (pure) NC gas improved

Quench front model applicable already at p < 5 MPa (former 3 MPa)

Length of plot array is printed in .out file

08.11.16 **Coupling of 3D neutron kinetics codes with ATHLET is done now exclusively via plugin technique. The 3D neutron kinetics code has to be provided by the user as DLL or shared library, resp.**

New input data check concerning definition of priority chains of autonomous systems

Processing sequence improved to enable identical results of serial and parallel execution of ATHLET

Several bugs / shortcomings of plotting package fixed

Print `'ARTIFICIAL EVAPORATION...'` does not longer appear for discharge junctions (JTYP=5)

Distribution of 64 bit code version only (32 bit version can be provided on request)

Intel Fortran compiler option "Floating Point Speculation" changed from *fast* to *safe*

Linux code version: change of Intel Fortran compiler from version 15.3 to 16.4

Several input / program checks improved / extended.

We recommend the download of the complete setup file and to re-install ATHLET.

15.07.16 ATHLET 3.1A Patch #01 released

Non-critical patch

14.07.16 Improved import and print-out of input OMP-settings (PW PARALLEL)

13.07.16 New error check for inconsistent input data: BRANCH2M coupling (i.e. JDPA=2) no longer possible for junctions, of which JDPA is set equal zero by BRANCHING data

12.07.16 Unix GUI, tool “Plot by plx file”: error in file selection dialog corrected

06.07.16 New tool to convert .plt to .plx files.

05.07.16 A GCSM summary is printed including number of loosely and closely coupled signals, external signals, etc. (s. NUMBER OF GCSM SIGNALS)

05.07.16 TFO component 'condenser' (ICMPO=4) may be a copy of standard TFO and vice versa.

04.07.16 Module CDR1D: Control of automatic update of CDR1D tables improved. It completes checks and avoids unnecessary updates.

29.06.16 Speed up of FEBE equation solver (identical results)

29.06.16 Discontinuity in calculation of HTCMIC removed; may speed up simulation

28.06.16 athlgo considers wall time and number of CPUs (OMP parallel execution of ATHLET) when limiting MCPU.

28.06.16 Check of external GCSM signals only on demand; may speed up simulation significantly if a very large number of GCSM signals is defined

24.06.16 Improved readability of TIME INTEGRATION SUMMARY print output for long term simulations (> 100000 time steps)

08.06.16 Check concerning applicability of quench front model (p < 30 bar) improved.

19.05.16 Parameter list of interface routine MHMASL includes now annular flow length, too. MASL calculation starts now at begin of transient calculation. Start values for transient MASL are no longer input data but results of stationary MASL.