Gesellschaft für Anlagen-
und Reaktorsicherheit
(GRS) gGmbH

ATHLET

Program Updates

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Gesellschaft für Anlagen-
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ATHLET 3.5

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About this Document

The ATHLET Program Updates Manual lists the major program modifications and patches to the current ATHLET code version. 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" in the *User's Manual* as well as under "Input Data Updates" in the *Input Data Description*.

On ATHLET patches: Although ATHLET is comprehensively tested and validated before it is released, program errors or weaknesses 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 the scope and complexity of 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 the ATHLET User Area. The user is strongly recommended to update his ATHLET version and recent results obtained with the previous code version.
- **Non-critical**: The code performance, predictiveness and/or user convenience are improved. Particular applications may require program updates which are not needed for usual applications.

Chap. 1 of this document summarizes the program changes and updates included in the current program version. Known issues in the code and their resolution or applicable workarounds are described in chap. 2. All further sections of the document provide information on program changes provided with former ATHLET code versions.

1 Program Updates in ATHLET 3.5.0

1.1 Thermo-Fluiddynamics

- Extended spacer grid model considering convective heat transfer enhancement downstream the spacer grid and droplet breakup in dispersed flow regime
- Dedicated friction loss correlations for TFOs coupled to a helically coiled heat exchanger HCO, applied on both sides inside curved tube and outside tube bundle
- New heat pipe module available, to be activated by PW `HEATPIPE` under CW `OBJECT`
- New model to calculate wall friction in the laminar and laminar-to-turbulent transition region. Further model options can be activated via new input parameter `ITRNS` under PW `FRICTION`.
- Limitation of bulk condensation rate (direct condensation model) at high void fraction and low liquid subcooling to avoid liquid superheat due to steam condensation.
- For collapsed level calculation (`ITML0=0` under PW `MIXLEVEL`): Print and plot data under keyword `MIXLEVEL` reduced to significant quantities
- Optional usage of centralized flow regime map module via parameter `AA` under CW `MISCELLAN`.
    - Comes with new print/plot output data denoting the flow regime; new parameters `IFLRI` (`IFLRJ`) for CV (junction) substitute former output parameters `IFL*`
- 3D TFO data derived from input under CW `TOPOLOGY` and PW `GEOMETRY`. More detailed 3D data can be defined with new PW `POSITION` under CW `OBJECT`. The data can be used for a 3D graphical representation of the fluidic network (vtk plug-in). The 3D data may be used by various models in future.
- New optional SW under CW `TOPOLOGY` for extended configuration control by switching on/off whole sets of PCs.
- New PW `SSCFRIC` under CW `OBJECT`: For priority chains with `IPRI0`>0 (adaptation of friction losses allowed), the adaptation of friction losses performed during the

steady state calculation (SSC) can be individually controlled for single TFOs or junctions.

- Additional print and plot data for mass and energy balances:
  - mass balance per TDV (keyword `TDVBAL`)
  - energy loss per TFD system (under `TFDGENERAL`)
  - mass balance per NC gas component per TFD system (under `TFDGENERAL/MCOMPBAL`)
- Mass balance output under `FLUIDBAL` for coupled calculations with COCOSYS/CFD corrected. Mass flows into/out of an external coupling branch (`ICOPLO`>0) are added either to `LEAKMASS`, if coupled junction is discharge or coupling branch is not a TDV, or to `TDVMASS`, if coupling branch is TDV.
- In order to avoid a program stop, the mixture level simulation is terminated, if the mixture level passes a not-integrated junction (e.g. a closed valve).
- CW `FORMLOSS`: pressure loss correlation for cross flow through a pipe bundle added
- Zinc-Borate transport and deposition models expanded:
  - Formation of mobile ZnB particles if Zn saturation concentration is exceeded
  - ZnB particle deposition at spacer grids up to blockage of flow channel
  - Deposition of ZnB on fuel rods and consideration of thermal resistance of ZnB layer for heat transfer calculation
- Unified calculation of onset of entrainment and entrainment fraction

1.2 Heat conduction and heat transfer

- New option to define a HCO that simulates a horizontally oriented plate located right above or below (or even within) a vertically oriented CV. The HCO consists of a single HCV. A dedicated HTC correlation (Churchill) for natural convection heat transfer at bottom/top of a plate is employed.

- HTC calculation under post-CHF conditions inside helical heat exchanger tubes uses Mc Eligot correlation; former implementation resulted in an program error if post-CHF heat transfer was reached.
- Print/plot output of `MODEL/R` corrected for heat transfer regime 21 (subcooled nucleate boiling)
- Extended radiation model enables radiation heat transfer between HCOs connected to different TFOs. Corresponding groups of radiation bodies can be defined under new KW `FLEXRAD`. The geometry and nodalization of the HCOs have to meet certain requirements.
- 3D data for HCO derived from geometry input of HCO and connected TFO. Can be used for 3D graphical representation.
- Optional 2D/3D solution of heat conduction for HCOs, can be activated via CW `HCOCONNECT`. Also enables heat conduction calculation between HCOs.
    - If activated, NuT is used for the solution of the heat conduction equation system.
- Each HCO may consist of more than three material zones. **Consider new meaning of input parameter `NADDMZ` in the HCO network and control data section!**
- Additional built-in materials available: `BORCARBIDE`, `INCONEL600`, `ALUMINA`
- For HCO with TFOs coupled on both sides (e.g. heat exchanger) the mutual assignment of HCVs and CVs has been improved to facilitate input data definition.
- Additional print/plot output for an HCO, whose surfaces (left and/or right) are coupled to a TFO with mixture level. For each mixture level, heat flows, HTC and other quantities related to the sub-CV above the ML are printed under the keyword `ML_LEFT` or `ML_RIGHT`.
- Calculation of thermal conductivity for liquid metal working fluids in Forster-Zuber HTC correlation corrected
- Thermal resistance of oxide layer (see PW `ZROXIDAT`) is considered for calculation of wall-to-fluid heat transfer. Currently, the heat conductivity of zirconium oxide is used, independent of the cladding material selected by parameter `MODOXI`.

Note: This program modification also affects existing input data sets that model an initial oxide layer via PW `ZROXIDAT`, parameter `ZROX0`.

1.3 Neutron Kinetics

- Average temperature `TRHOEXP` of CVs (or HCVs) for calculation of thermal expansion feedbacks provided as output quantity. Only CVs (HCVs) with a form factor greater than zero are considered.

1.4 Numerical Solver

- Numerical Toolkit version increased to NuT 2.1.0 (for details see NuT documentation)
    - Enables local use of NuT; however, use of NuT worker (separate process) is still possible
    - By default, solution of 3D heat conduction in structures (CW `HCOCONNECT`) and inventory calculation by VENTINA make use of NuT's local interface and dedicated algorithms.
- Modified effective local error bound derived from the absolute and relative error bounds

1.5 Component Models

- Critical discharge model CDR1D: new option via `IAUR=+/-5` to consider phase drift in evaporation and condensation model. Activation of extended CDR1D model changes meaning of input parameters `TURB` and `CMUEK`.

1.6 GCSM

- Additional input check for `FUNGEN` controller without `X2NAME` specified: `IOPT` must be -2 or 0 (other options for `IOPT` cause a program stop)
- Re-ordering of GCSM process signals during input processing to increase code efficiency

1.7 Plug-ins

- Extension of convective heat transfer plug-in `MTHCEXT_CONVECTION` to film boiling heat transfer regime
- Interfaces in `MHTCEXT` plug-in updated
- MASL plug-in provides additional options to control stationary MASL and thermal margin
- New plug-in `vtk` for output of 3D TFO and HCO data using the format vtk (for visualization e.g. with ParaView)
- Plug-ins for CHF calculation, `MHCHFEXT` and `MHCHFEXT_EXTERNAL_FLUID`: index of inlet CV of core channel added to parameter list. This facilitates the access to core entrance flow conditions to be used in the user-provided CHF correlation.
- Update preCICE adapter to current preCICE version 3

1.8 General

- FMU controller to couple ATHLET with MODELICA-based models
- New output quantities under keyword `MONITOR`:
    - `IJLIM`: time step size limiting CV or junction
    - `IJRED`: time step size reducing CV or junction
- ATHLET internal time variables transferred to real(16); output format is still real(8)
- New sample sample1_vtk.in including 3D TFO data
- Input under CW `COCOSYS`, PW `COUPLING` changed: a user-defined name `ACPLNAM` for print and plot output has been added and `S0INP` has been removed
- Print output of `MODEL/R` for heat transfer mode 21 (subcooled nucleate boiling) corrected
- Some models originating from ATHLET-CD have been integrated in ATHLET:
    - VENTINA for initial inventory calculation and decay of isotopes

   - FPREL and SAFT for release, transport and deposition of radionuclides in LWR
   - THEMEC for fuel rod behavior, ballooning, and feedback on thermal-hydraulics (blockage)

- The output file named <input-name>*_EXP* is saved in the working directory instead of the input directory
- Output file <problem-id>*.minmax* including minimum and maximum values of plot variables removed
- HCO nodalization data (`N10` etc.) written to gr-file (used e.g. by batchplot)
- New optional input data check to detect unused parameters; check can be activated by new PW `IDLE_PARAM` under CW `SERVICES`
- Additional output quantity for mass residuum per CV
- All subroutines have been put into submodules with interface declaration to enable additional compiler checks for consistency

1.9 Tools

- Batchplot extended to visualize 2D SVG images generated by AIG
- The output format of the key file was modified so that very large systems with many output quantities can be properly handled.

2 Known and Fixed Program Errors

Tab. 2.1 lists major known bugs and shortcomings that are existent in the current ATHLET 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.

Tab. 2.1 Known Bugs in the current program version

Bug Description	Detected in code version
Restart error In rare cases, results of start and restart runs may numerically differ. This seems to be related to the code-internal conversion of the time variable from real(8) to real(16). Measures: None	3.5
Multicomponent model: Mass error in NC gas balance equations Various gas components can be activated under CW `MULTICOMP` and simulated in one or several TFD systems. But even if a specific gas component cannot appear in a particular TFD system due to physical reasons, small amounts of this gas component can be generated by ATHLET due to round-off errors. It is expected that the impact on the physical simulation results is small. However, the numerical performance of the code might be impaired.	3.3
Multiple parallel channels with MLs: Numerically unstable behavior Particularly for parallel channel models, multiple parallel MLs can behave unstably at least for (pool) boiling situations. Numerical issues may also lead to unphysical behavior. Parallel mixture levels repeatedly transitioning CV boundaries at same elevation can also impair numerical efficiency. Measures: For pool boiling situations a final solution is not available. In general, the ML transition criteria under PW `MIXLEVEL` can be optimized, or the CV boundaries can be changed so that (slow) ML transition is avoided.	3.2 (and former versions)
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 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).	3.1A

3 Patches for ATHLET 3.4.0

The following lists the ATHLET program patches for the release version ATHLET 3.4.0.

In this chapter, **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.

01.04.25 ATHLET 3.4.3 released, non-critical patch

28.02.25 **Properly set unassigned variable `SQH14` (upper enthalpy limit used for CHF correlation); this code modification impacts and corrects the CHF calculation in following cases:**
- if pressure rises above 219 bar (up to critical pressure) and working fluid is water
- if CHF plug-in is used (independent of selected working fluid)

19.02.25 CHF plug-in for external fluid: order of command line parameters provided to plug-in subroutine `MHCHFEXT_EXTERNAL_FLUID` corrected.
CHF plug-in for water as working fluid: INTENT statements corrected

Note: Since the code changes related to this patch ATHLET 3.4.3 do not impact the results for the validation tests presented in the Validation Manual, the code documentation remains unchanged compared to ATHLET 3.4.2.

25.11.24 ATHLET 3.4.2 released, non-critical patch

25.11.24 Coupling with COCOSYS via PW `COUPLING`: If the coupling branch was defined as TDV in ATHLET, physical quantities provided by COCOSYS to ATHLET (e.g. pressure) were not transferred properly. The implementation has been corrected and a TDV may be a defined as coupling branch now. In addition, mass balances given under `TFDGENERAL` have been corrected for coupled calculations. This applies to couplings using PW `COUPLING` or CW `EXT`.

15.11.24 Batchplot plotting tool: Batchplot's 'ac2.athlet' package does no longer rely on the information provided by .gr and .key files but reads geometry and unit information from the HDF5 output file instead. Consequently, HDF5 files generated with ATHLET version earlier than 3.4.0 are now rejected by ‘ac2.athlet’ as they do not contain this information yet.

15.11.24 For Moody and HEM critical flow models: interpolation in critical discharge table corrected

30.09.24 Improved and extended input data error checks

30.09.24 `MHTCEXT` plug-in: sample data set added to test the plug-in; sample routines added to demonstrate how to calculate working fluid properties for both liquid and vapor

13.09.24 Maintenance update of hdf5 package to version 1.14.2, mainly to improve performance and to benefit from security fixes

17.05.24 ATHLET 3.4.1 released, non-critical patch

17.05.24 Correction in compact heat exchanger model (PW `HTEXDEF`); wrong indexing could cause error in heat transfer and pressure drop calculation

15.04.24 Fuel rod gap model: Correction of gap volume, used for calculation of gap pressure

07.03.24 The variable `DMTMS`, which is the molten mass of heat structures (ATHLET-CD), has been added to the restart file. Hence, the restart file format changed, so that restart files of the ATHLET versions 3.4.0 and 3.4.1 became incompatible.

07.03.24 CW `INTEGRAT`, PW `DEBUG`: Corrected print output of partial derivatives (for debugging purposes only)

05.02.24 Output Description (part 5 of the ATHLET User’s Manual) improved: The output level, which refers to the parameter `IOUT0` under CW `OBJECTCON`, has been added to the description of each output variable.

19.01.24 The flow regime index `IFLVS`, which is only printed and used for post-processing purposes, has been corrected.

4 Program Updates in ATHLET 3.4.0

In this chapter, **bold face** indicates that user's action may be required even for existing input decks.

4.1 Thermo-Fluiddynamics

- Dedicated form loss correlations for bend and contraction. The correlations can be invoked using the new CW `FORMLOSS`.
- New CW `FORMLOSS` for specification of Re-number dependent flow losses via input table.
- 3D-model combined with mixture level model, e.g. for the simulation of water pools: The momentum flux calculation for horizontal flows at mixture level elevation (i.e. for junctions connected to CVs including the mixture level) has been modified, so that full acceleration loss is calculated now.
- Pressure drop correlations for plate heat exchanger geometry. The model is activated by the new PW `HTEXDEF` under CW `STEAMGEN`.
- CoolProp fluid properties library coupled via controller approach. An example python controller script is part of the AC² distribution.
- For T-junctions: pressure loss/increase in main pipe considered for 2M (6-equation) model.
- T-junction model also applicable together with 2M model (validation is on-going).
- Improved implementation of subcooled boiling at low void fraction to mitigate mass conservation error
- Initialization of arbitrary NC gas mixtures in single TFOs and complete TFD-systems enabled (new PW `INITXVNC` under CW `MULTICOMP`)
- Solute transport model considers maximum filter capacity for removal of solute component
- Slightly modified bulk condensation model: now, the penetration depth is non-iteratively calculated using the HTC from renewal theory; in addition, a new option

IGVK=5 has been introduced to calculate the penetration depth by the Gilliland and Sherwood correlation.

4.2 HECU

- New heat transfer correlations for helically coiled heat exchanger: The model can be activated by the new PW HTEXDEF under CW STEAMGEN.
- Multiplication factor OHWFC for convective heat transfer to liquid (CW MODELUNC – for uncertainty and sensitivity analyses) is used for all working fluids now (was restricted to water and sodium before).
- Corrected bundle factor calculation for hexagonal bundles acc. to Inayatov. The correlation for hexagonal bundles is consistently used in all heat transfer levels now.
- New CHF correlation proposed by Song et al.: Can be activated by input parameters ICH1 and ICH6.
- Optionally, user-defined SW (S----) may be used under CW HEATCOND to group the HCOs. This option can be used to easily switch on/off a group of HCOs.
- Heat transfer correlations for plate heat exchanger. The model is activated by the new PW HTEXDEF under CW STEAMGEN.
- A radial power distribution inside the power generating material zone of a rod can be optionally specified using the new PW RADPOW.
- New correlations for the simulation of austenitic and ferritic steels oxidation
- **Extended input checks: Power profile under CW ROD has to be provided for the complete length of the HCO.**
- **New input check under PW ZROXIDAT for ATF. The lower temperature boundary OXTCB must be provided first, before the upper boundary OXTCE is input. Thus, the input order basically changed, but is in accordance with the input description now.**

4.3 Neutron Kinetics

- The deprecated 1D neutron kinetic model was removed.

- Point kinetics: The structural moderator model to consider e.g. the graphite matrix in pebbles was fixed. The old implementation did properly run for only one single rod component.

4.4 Numerical Solver

4.5 Component Models

- Heat exchanger model: Using the new PW `HTEXDEF` under CW `STEAMGEN`, additional data can be provided to specify the geometry of a plate heat exchanger. Dedicated models will be employed for heat transfer and pressure drop.

4.6 GCSM

In addition to water, the controller `GPROP` can be applied now to other boiling working fluids (sodium, potassium) as well.

4.7 Plug-ins

- HDF5 writer plug-in supports SWMR (Single Writer Multiple Reader) mode now. That feature can be activated via -swmr command line argument or AC2_USE_SWMR environment variable. In general, the SWMR mode enables writing and reading an HDF-5 file in parallel. By default it is false. Not supported by ATLASneo yet.
- The interface for heat transfer to supercritical water included in the MHTCEXT plug-in has been modified. Additional parameters are provided to the routine MHTCEXTSC: bulk viscosity, specific heat capacity and heat conductivity (can e.g. be used to calculate Re and Pr numbers)
- The interface for convective heat transfer to liquid included in the MHTCEXT plug-in is no longer limited to the working fluid water but can be used for any working fluid to employ external htc correlations.
- MHCHFEXT plug-in for user-provided CHF correlations extended by an interface routine for ‘external fluid’, invoked by the CoolProp library.

- MHTCEXT plug-in: interface `mhtcext_pdo` for user-provided film boiling htc correlation added. User-provided HTC correlation can be invoked by `IHTC1L/R`<0 or `IHTC2L/R`<0.
- The MHTCEXT plug-in was corrected, so that it can be employed together with the parallel program version, too.
- Updated hdf5-writer plug-in with new CMake-file, required due to compatibility issues with ATHLET-CD and COCOSYS

4.8 General

- HDF-5 file expanded by units for plot variables and TFO / HCO geometry data.
- Unit information for process signals added to key-file (used by ATLAS).
- Restart data have been expanded, e.g. by data required for Reynolds number dependent form losses and by GCSM control signal parameters `IOPT`, `GAIN` and `A1` to `A4`. As a consequence of this, restart data files generated with former ATHLET versions aren't compatible and cannot be used together with ATHLET 3.4.
- Input data deviations from recommended values according to the Input Data Description are written to the .log file.
- Compatibility mode to start ATHLET with both arguments problem-ID and run-ID (the standard command line syntax of ATHLET 3.1 and earlier code versions) was removed.
- The names of some plot variables have been changed. Changes refer to names that included a backslash, which was mainly used for some NC gas variables. The backslash was substituted by an underscore. E.g.: `RMVMC/001` has been changed to `RMVMC_1`. As can be seen, leading zeros have been omitted as well for better readability. Please adjust existing post-processing files (design or .atl files), if one of the modified variable names is used.
  The changes became necessary, since a slash is typically used in the hdf5 format as string separator.
- **The use of following characters has been forbidden for object names, GCSM signal names and GCSM block names: '/', '\', '%'**

- Improved “Minor Time Step Edit”: The print output per time step provides information on the differential equation or physical model responsible for a time step limitation and now includes information from ATHLET-CD as well.
- **Input format under CW `MIXLEVEL` has changed: if more than one mixlevel is defined for one TFO, the two records for the first mixture level have to be input before the two records for the second ML and so on (instead of first input record alternating for all ML before second input record alternating for all ML, as it was before).**
- Recalculation of CDR1D critical discharge tables: The decision to recalculate the tables is now taken on the basis of a string-to-string comparison (instead of a numerical comparison) between the input under CDR1DIN and CDR1DTAB. This ensures the recalculation also in case of only small changes to the input values.
- Extended input checks on validity of provided `IHTC*L/R` options.
- The print output was improved, so that the name of the used CHF correlation is given now. The name was missing so far, if the correlation was employed beyond general validity bounds defined in ATHLET (print output “outside limits”).
- **Extended input error checks**: The syntax of the input deck has to be in accordance with the input data description. Now, the input deck is widely checked for validity and order of KW and/or PW given under the various CW available for ATHLET (and ATHLET-CD). Spurious input is detected.
- New PW `PRNT_INPUT` under CW `SERVICES` available to control the output of the input data set with parameters substituted by their values.
- Control print and plot data amount under GENERAL, MONITOR and TFDGENERAL by the input parameter `IOUT0` (CW `OBJECTCON`)
- Refactoring and removal of Fortran statements declared as obsolescent in Fortran 95 to prevent compiler warnings
- Option `PLOT_SSC` enabled for datasets that doesn’t include any HCO
- Output at the end of the .out-file with regard to FEBE statistics expanded
- Optional user-defined SW under CW `PARAMETERS` to structure and switch-on/off parts of the parameters section

4.9 GUI / Tools

- Outdated GUI for ATHLET software tools under Linux has been removed. The tools are still accessible from the command line.

5 Patches for ATHLET 3.3

The following lists the ATHLET program patches for the release version ATHLET 3.3.

In this chapter, **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.

04.10.22 ATHLET 3.3.1 released, non-critical patch

01.06.22 If dedicated heat transfer correlation for condensation in vertical pipes (input option `IHTCI(4)=11`) is used, the final condensation HTC is calculated as maximum out of condensation HTC and convection HTC now. This keeps the convective heat transfer as minimum and avoids the HTC tending to zero e.g. if condensation is reduced due to NC gases.

30.05.22 SBTL95 plug-in uses IERR return value for error handling.

30.05.22 Refactoring of the routine DIMC, which is responsible for parsing the input under CW `MULTICOMP`. The refactoring also enables TFO names that include a slash ("/") as a character, which was already possible through all other sections of the input deck.

10.05.22 Slight modification of momentum flux term (2M-model) in case of a disappearing phase.

28.04.22 For gas component `AIR-N2O2` (newly available in code version 3.3): **Initialization of Nitrogen and Oxygen mass fractions after SSC corrected.**

15.03.22 MTHCEXT plug-in extended by additional interfaces for user-provided HTC correlations for convective heat transfer to liquid and/or vapor (for both cooling and heating surfaces).

11.02.22 Improved implementation to avoid negative entries for CPU time in the "CPU STATISTICS" printed at the end of the print output file (relevant for long running jobs only)

26.01.22 VVER-1000 sample case: use mixture level model in steam generator hot and cold collector pipes

24.01.22 **GCSM predictor-corrector integration corrected**: The block-specific setting `INTEK=2` resulted in an erroneous calculation of controllers of types `SWITCH`, `TSSWITCH` and `INTE` used in the respective GCSM block.

24.01.22 MTHCEXT plug-in extended by an interface for user-defined HTC correlation for condensation heat transfer. The plug-in is activated by the input parameter `IHTC4L/R` (under CW `HEATCOND`).

Tools:

ATLAS: Distribution plots available again via the dropdown menu for the variables in the keyword list (instead of the option “Shapiro-diagram” that was erroneously listed in the dropdown menu)

AIG-2: Several patches are provided:

- Possible program crashes during the import of faulty or incomplete GR files are intercepted now.
- The graphic errors which occurred during the representation of TFO - HCO objects parameterized in opposite directions and during the representation of the schematic TFO network were eliminated.
- The arrow for displaying "twisting at point" is hidden in the updated AIG2 version either when changing the TFO on the surface or when closing the specific mask.
- The obsolete error-file output and automatic SVG file output functions were removed.

6 Program Updates in ATHLET 3.3

In this chapter, **bold face** indicates that user's action may be required even for existing input decks.

6.1 Thermo-Fluiddynamics

- New evaporation model for mixture level with a more realistic consideration of impact of NC gases
- Modified ML condensation model
- Improved modelling of entrainment fraction (based on Pan-Hanratty) and of onset of entrainment for horizontal pipes
- 3D model: if TFO is part of a 3D (cylindrical) domain and annulus drift is specified in the input, pipe drift will be used instead
- Additional transport equations for solutes (mainly thought for analysis of zinc-borate issue after LOCA)
- Modelling of zinc release from internals (for gratings in containment)
- New vertical bundle drift option for small-size test facility bundle
- New gas components available: CO and CO_2
- Special treatment of arising/vanishing phase (i.e. very small phase fraction) in momentum equation removed (subroutine D2MDZC)
- Updated thermodynamic properties of NC gases. In order to ensure consistency, specific gas constants are now calculated from molecular weights.
- If *reduced* input format under PW `MIXLEVEL` was employed, `AMLSO` and `VMLTO` weren't correctly interpreted. Fixed.
- Correction of evaporation rate due to overheated steam according to Sideman. Factor $1 - \gamma$ omitted.
- Adaptation of boron transport model
- Calculation of flow losses in bulk condensation model corrected.

- Bug-fix in Double-end-break model. Model was not executable in previous code version.
- Modified formulation of so-called water-level force (2m)

6.2 HECU

- Flow instability ratio acc. to Whittle-Forgan as optional plot quantity (print level `IOUT0`=4) (mainly for research reactors)
- Cladding oxidation model extended for FeCrAl (ATF)
- New CHF correlation acc. to Sudo and Kaminaga, mainly for research reactors and fuel assemblies with narrow rectangular flow channels
- If wall temperature exceeds Leidenfrost temperature, a modified fluid reference temperature for calculation of heat transfer is employed
- Dedicated heat transfer correlations for thermosiphons acc. to Gross (condensation) and Imura (evaporation) implemented (selectable via input parameters `IHTC4L/R` and `HTC7L/R`, resp.)
- **Meaning of `TL0` (fuel rod pitch) extended to distinguish between square and hexagonal bundles** (e.g. required for Inayatov bundle factor)
- Special heat transfer correlations for laminar, wavy and turbulent film condensation within vertical tubes, selectable via input parameter `IHTC4L/R`
- Slightly modified calculation of transition boiling heat transfer in order to enable earlier rewetting for those HCVs that didn't reach film boiling before

6.3 Neutron Kinetics

- Additional thermal-hydraulic feedback reactivities available, mainly for LM cooled reactors: thermal cladding expansion feedback, thermal fluid or structure expansion feedback for any TFO or HCO

6.4 Numerical Solver

- NuT – if activated – is used during SSC as well

6.5 Component Models

- Condenser model with NC gases: Condensation of inflowing vapor is limited to saturation pressure at present liquid temperature.
- Separator model: For flooded separator and ML inside the dome, the distribution of carry-over steam mass flow is adjusted. Non-separated steam is directed to lowermost CV (below mixture level) of separator dome instead to separator exit branch.
- Separator model: The distribution of separated carry-under liquid mass flow below/above mixture level in separator outlet branch is corrected. Former implementation could result in (low frequency) oscillations of the mixture level in the separator outlet branch.
- **Injection model: injection angle `ANGINJ` for injecting TFO is limited to $0 \leq ANGINJ \leq 180$: (for ECCMIX injection: $0 < ANGINJ < 180$)**
- Time-Dependent Volume (TDV): New optional input (PW `CORRLIMIT`) to limit or skip pressure and enthalpy adjustments after SSC

6.6 GCSM

- New GCSM postprocessing signal (via CW `POSTPRO`): total fluid enthalpy in TFO
- Additional call of GCSM at the end of SSC to correctly set process signals related to NC gas quantities. Hence, all control signals will be updated too.
- **For CV with mixture level inside, the process signal type `PRESS` provides now the pressure in the center of the CV and no longer the pressure at mixture level elevation.**

6.7 Plug-ins

- New plug-in for water-steam material properties according to IAPWS-95 standard with increased accuracy mainly in the range of low pressure (≤ 1 bar). Plugin is activated under CW `PLUGIN` writing “sbtl95” and is employed if light water is working fluid.
- **Initialization of plug-ins is shifted to the beginning of an ATHLET run, when CW `PLUGIN` is read in**

- Additional non-boiling model working fluids added to plug-in MPEXT.
- MHTCEXT plug-in extended by additional interface for *forced convection heating to liquid* heat transfer regime
- Coupling via HCO-surface (e.g. with COCOSYS) improved
- Gain-factor for GCSM signals of type `EXTERNAL` no longer used
- ATHLET Water-Steam property package available inside plugin MHTCEXT
- CFD coupling interface expanded to NC gases
- To handle different 3D neutron kinetic code plug-ins in parallel, the naming convention for the according libraries was modified. The library name must start with “n3kin” and may be expanded additional characters, e.g. “n3kin_dyn3d”.

6.8 General

- Restructuring of loops in routine DGZON to reduce CPU time
- Intel Fortran 19 compiler used for current release
- Restart format modified: old restart files will not run with current program version
- Jacobian coherency test implemented (developer tool): to be activated via environment variable ATHLET_CHECK_JACOBIAN_COHERENCY (for both MS Windows and Linux)
- Plot data for models NEUKINP, STEAMGEN and QUENCH are provided independently of HECU output amount (e.g. if `IOUTH0`=0)
- New print/plot data: flow regime information from both interfacial shear model as well as heat and mass transfer model
- libadt.dll is replaced by libfde.dll

6.9 GUI / Tools

- New python-based plotting tool ‘batchplot’ available
- Windows tools “Plot Variable by Excel” and “Excel to pd” no longer distributed due to license constraints

- Several minor bug fixes and improvements in AIG
- Visualization error of mixture level in ATLAS within pipes with more than eight CVs fixed
- Output of the two post-processing utilities “Select Plot Data” (for MS Windows) and “athpost” (Linux) adjusted and harmonized to each other: e.g. a headline with variable names is always printed and the number of records is given in the first column.

7 Patches for ATHLET 3.2

The following lists the ATHLET program patches for the release version ATHLET 3.2.

In this chapter, **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.

03.06.20 ATHLET 3.2.1 released

Non-critical patch

03.06.20 New (optional) hardware-action to control point-kinetics rod power during zero-transient calculation. This option facilitates establishment of an asymmetric core power distribution, e.g. by initially specifying a homogeneous power distribution (also for the connected steam generators) and by adjusting this power distribution via GCSM during zero-transient.

Modified (optional) input data under PW `RODCON`:

Input:

```
IQF10 AIQF10 AIQF20 IPOWM0 IPOWL0 QROD0 QROD00 FPROD opt.:AQROD0
```

`AQROD0`: Optional input: Name of GCSM signal controlling relative rod power during zero-transient calculation (100% power: `QROD00`)

19.05.20 Bug fix for Dobson-Chato heat transfer correlation (condensation in horizontal tubes). Transition criterion between stratified and annular flow included an error.

27.03.20 Extended error checks for PW `BRANCHING`:

Branching data provided twice for one TFO (e.g. for a SJP connecting two branch objects) are checked for consistency

26.03.20 New process signals `TMTCORE` (average temperature of in-core melt) and `LPTWOAVE` (average outer surface temperature of the lower plenum [K]) are available (ATHLET-CD).

17.03.20 Spray model: print and plot variables `GAMDRO` and `HTCOUT` were not properly set.

24.01.20 Mismatch between Jacobian matrix structure (representing the thermal-hydraulic network structure on a matrix level) and the actual dependencies of solution variables according to physical modelling resolved. Comparing the patched code version with the original release version 3.2, this may cause (numerically) different results in cases where separator model, injection model, 3D model or the flag `I2MFTRX=1` is used. `ISFTRX` is always set to one now.

18.12.19 Additional trigonometric functions available under CW `PARAMETERS`: `arcsin`, `arccos` and `arctan`

12.08.19 Bug-fix in selection of heat transfer correlation for film boiling. Selection of Condie-Bengston correlation via input parameter `IHTC1L/R` resulted in program error.

12.08.19 Extended error checks w.r.t. priority chains provided by user

12.08.19 sCO_2 properties: Error in calculation of partial derivatives fixed

8 Program Updates in ATHLET 3.2

In this chapter, **bold face** indicates that user's action may be required even for existing input decks.

8.1 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`).

8.2 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)

8.3 Neutron Kinetics

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

8.4 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)

8.5 Component Models

- Separator-model: Corrected enthalpy flow rates across carry-under/over junction for cases with NC gases.
- New heat exchanger option for SSC: `IQHTX=2` iterates heat exchanger power profile but doesn't adapt heat exchanger 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).

8.6 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

8.7 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.

8.8 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)
- New simple sample: ATHLET "egg boiler"
- 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.

8.9 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)

9 Patches for ATHLET 3.1A

The following lists the ATHLET program patches for the release version 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 release

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.