New Models and Features in ATHLET 3.4.0

AC² User Meeting

27.11.2023, GRS Garching

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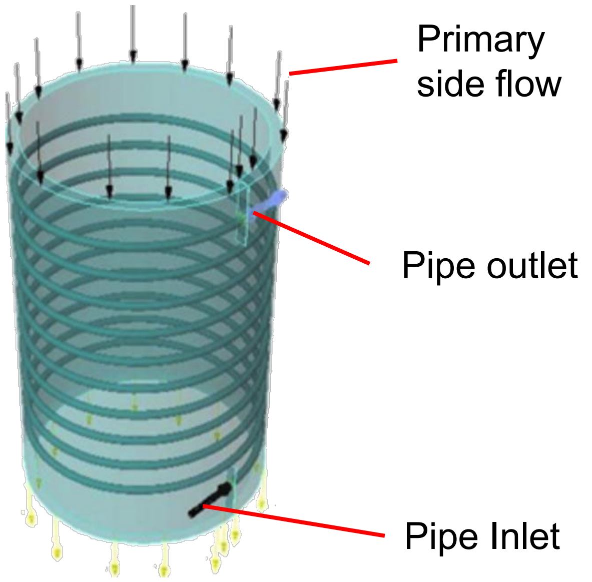
Content

- New and Updated Models in ATHLET 3.4.0
  - Modelling of Compact Heat Exchangers
  - Reynolds Number Dependent Form Loss Calculation for Specific Geometries
  - Extended Fuel Rod Model
  - New Working Fluids and Improved Multicomponent Model
- Further Program Improvements, New Input Options and Output Data
- Conclusions

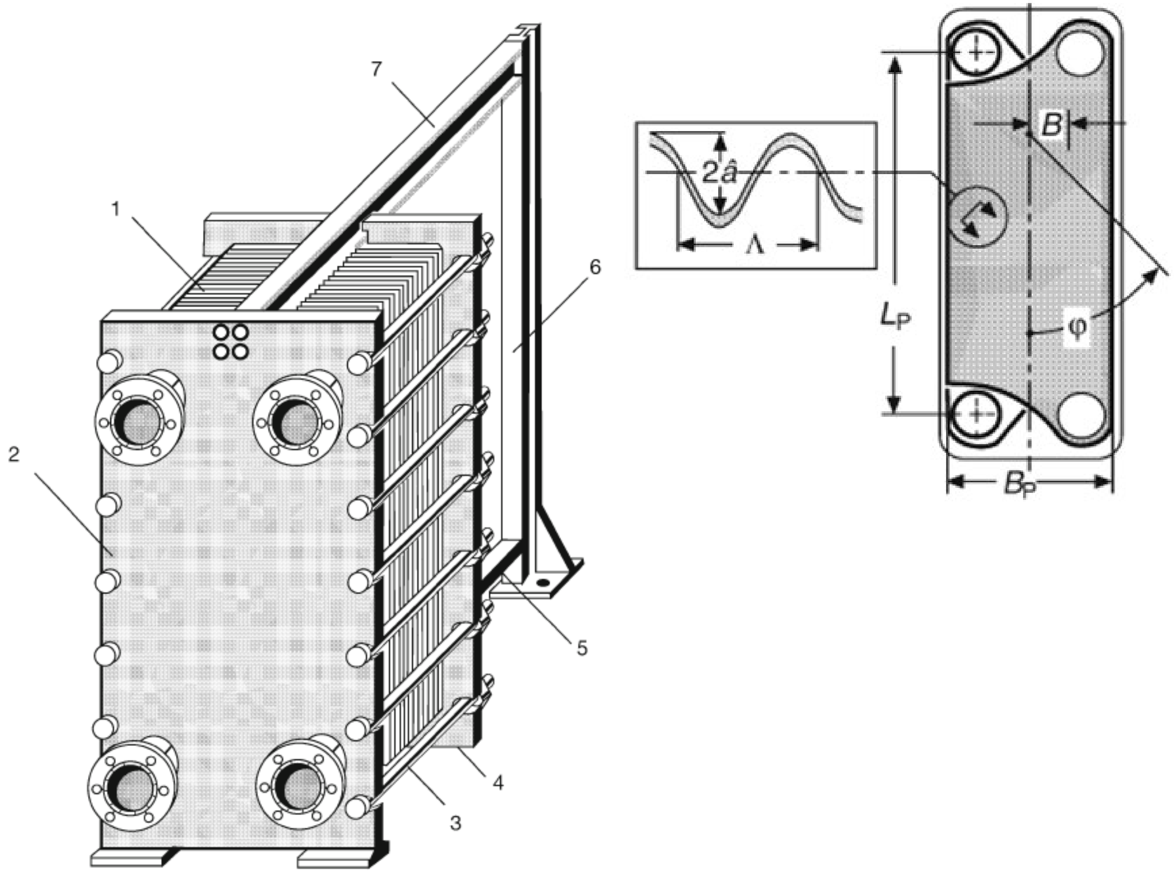
Component Model for Specific (Compact) Heat Exchanger Designs

Motivation: Innovative SMR concepts

- New designs of individual components such as compact heat exchangers
  - Little space required
  - High heat flux density
- NUWARD: Usage of **plate heat exchanger**
- NuScale: **Helical coiled heat exchanger**



Mikko Niemi: Simulation and safety features of NuScale small modular reactor, Master Thesis, 2017.



General design of a plate heat exchanger[1]

[1] Verein Deutscher Ingenieure (VDI), VDI-Gesellschaft Verfahrenstechnik und Chemieingenieurwesen (GVC): VDI-Wärmeatlas, Mit 320 Tabellen. VDI-Buch, 11. Aufl., 1760 S., ISBN 978-3-642-19981-3, DOI 10.1007/978-3-642-19981-3, Springer Vieweg: Berlin, 2013.

Implemented Correlations for Plate Heat Exchanger

- Correlation for **pressure loss for single-phase** flow (according to Martin/VDI[1]):

$$\Delta p_{fric} = \lambda \cdot \frac{l}{d_h} \cdot \frac{\rho w^2}{2} \quad \text{with} \quad \lambda = f(Re, \varphi),\ \varphi = \text{Chevron angle}$$

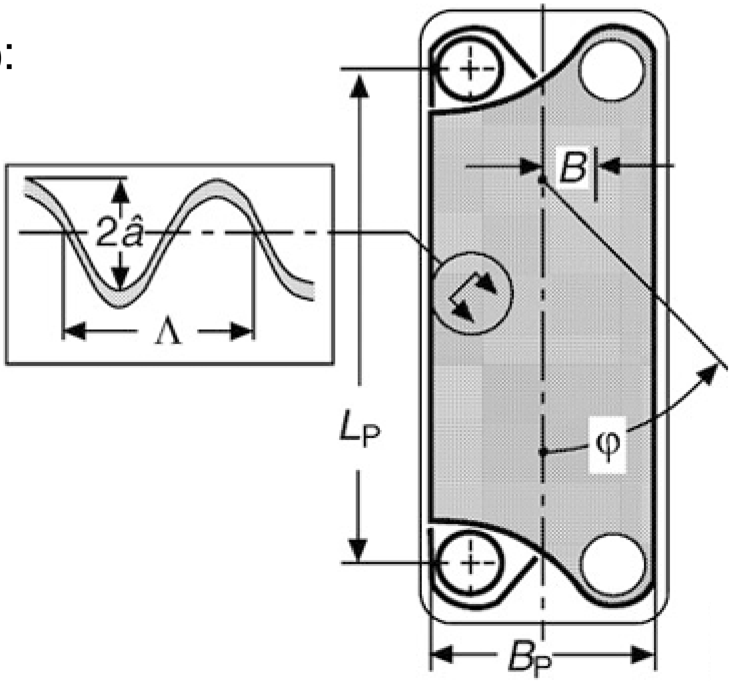
- Correlation for **pressure loss for two-phase** flow (according to Huang[2]):

$$\Delta p_{fric} = f_{tp} \cdot \frac{l}{d_h A^2} \cdot \frac{G J^2}{2\rho_m}$$

$$f_{tp} = \frac{3.81 \cdot 10^4\, F_{R,f}}{Re_{tp}^{0.90} \left(\frac{\rho_l}{\rho_v}\right)^{0.16}}$$

f_{tp}: Two-phase friction factor

$F_{R,f}$: Geometry parameter



- Specific HTC correlations for convection, condensation and evaporation (Huang[2]):

$$htc_{evap} = 1.18 \cdot 10^{-4} \cdot \left(\frac{\dot{q} D_h}{\lambda_l T_{sat}}\right)^{0.67} \cdot \left(\frac{r D_h^2 \rho_l^2 c_{p,l}^2}{\lambda_l^2}\right)^{0.42} \cdot \left(\frac{\rho_l}{\rho_g}\right)^{-0.1} \cdot Pr_l^{0.31}$$

[1] Verein Deutscher Ingenieure (VDI), VDI-Gesellschaft Verfahrenstechnik und Chemieingenieurwesen (GVC): VDI-Wärmeatlas, Mit 320 Tabellen. VDI-Buch, 11. Aufl., 1760 S., ISBN 978-3-642-19981-3, DOI 10.1007/978-3-642-19981-3, Springer Vieweg: Berlin, 2013.

[2] Huang, J.: Performance Analysis of Plate heat Exchangers used as Refrigerant Evaporators. University of the Witwatersrand: Johannesburg, August 2010.

Correlations for Helical Coiled Heat Exchangers

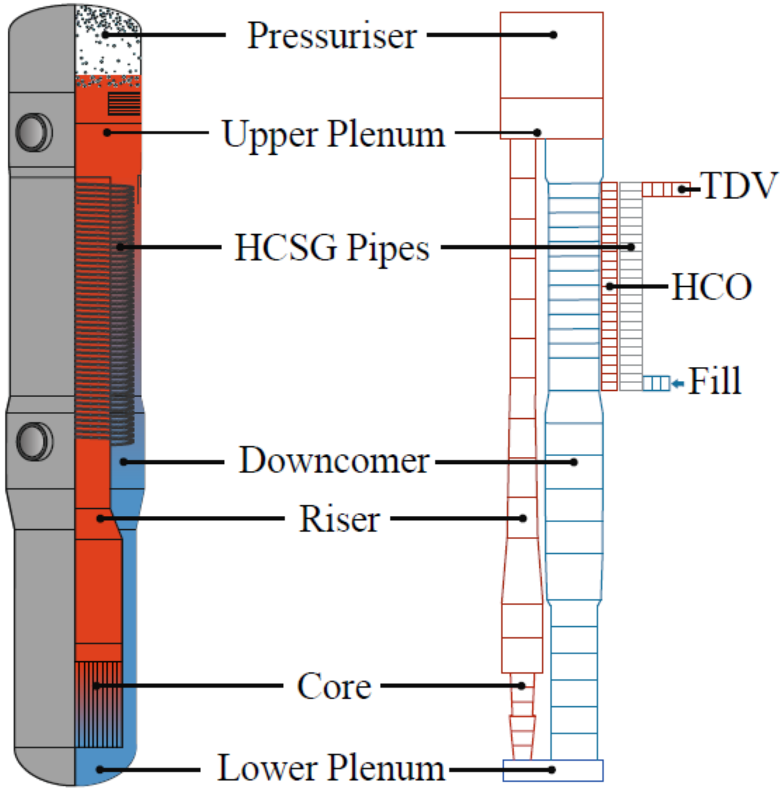
- HTC correlations for **convective heat transfer to liquid and vapor according to Mori & Nakayama**[1]

$$Nu_{Mori,liquid} = 0{,}023 \cdot \left(1 + \frac{0{,}061}{\left(Re \cdot \left(\frac{D}{d_c}\right)^{2{,}5}\right)^{\frac{1}{6}}}\right) \cdot \left(\frac{D}{d_c}\right)^{\frac{1}{12}} \cdot Re^{0.833} \cdot Pr^{0{,}4}$$

- Modified Chen HTC for two-phase flow, using Nu_{Mori} as macroscopic HTC
- **Shell side bundle heat transfer to liquid according to Zukauskas**[2]

$$Nu_{Zukauskas} = C(s_v, s_t) \cdot Re_{max}^{m} \cdot Pr^{n} \cdot \left(\frac{Pr}{Pr_w}\right)^{0{,}25}$$

- Model implementation and initial validation by RUB/Krieger



Krieger et al.: Simulation of the experiment OSU-002 regarding the behavior of a helically coiled steam generator using AC²-ATHLET, ICONE30, 2023

[1] Mori, Y., Nakayama, W.: Study of forced convective heat transfer in curved pipes (2nd report, turbulent region). International Journal of Heat and Mass Transfer, vol. 10, no. 1, pp. 37–59, DOI 10.1016/0017-9310(67)90182-2, 1967.
[2] Zukauskas, A.: Heat Transfer from Tubes in Crossflow. Advances in Heat Transfer, vol. 8, pp. 93–160, DOI 10.1016/S0065-2717(08)70038-8, 1972.

Input data for compact heat exchangers

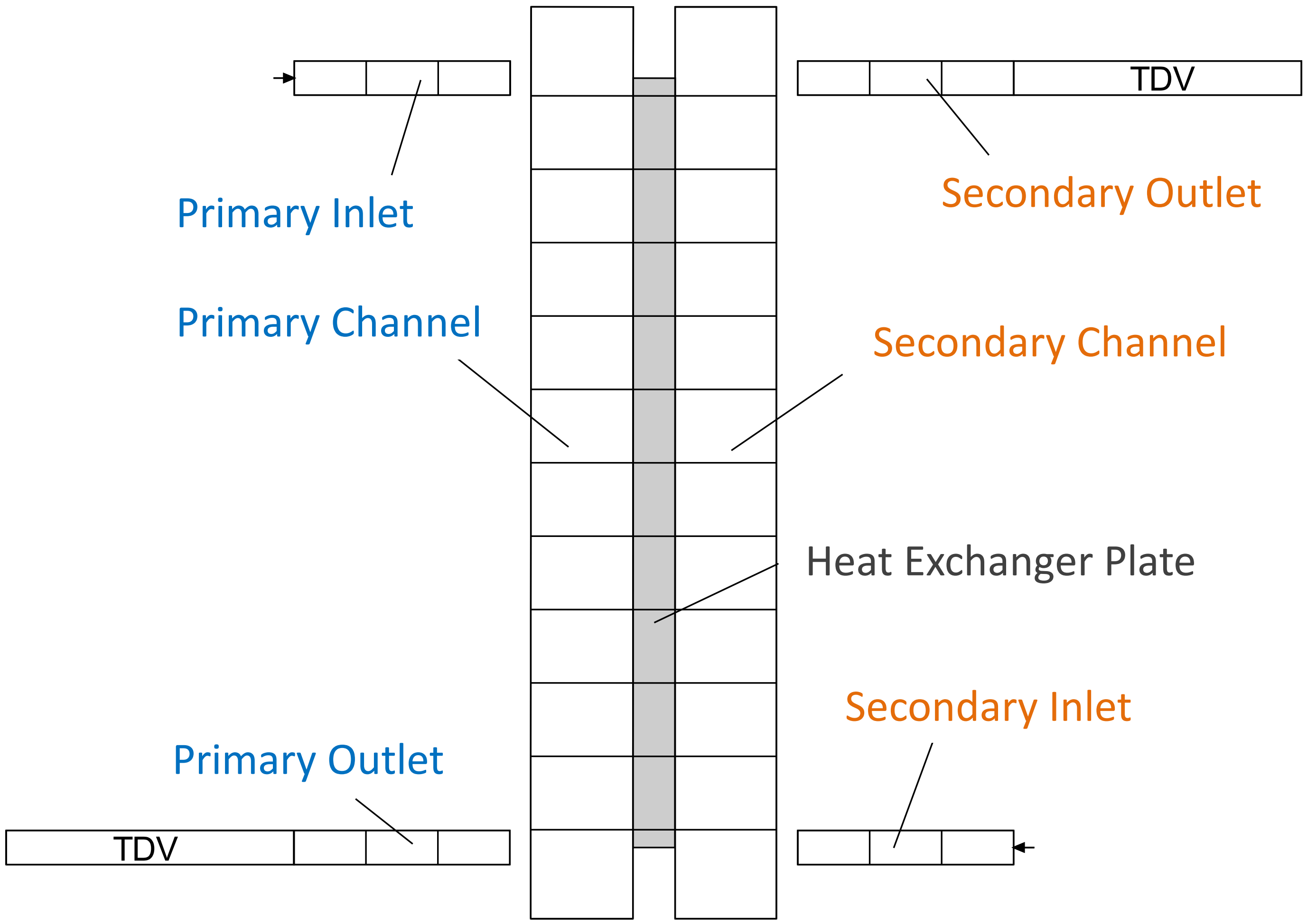
- CW `STEAMGEN` using the new PW `HTEXDEF`
  - `IHTEXTYP`: **Type of specific heat exchanger**
    - = 1: Plate heat exchanger
    - = 2: Helical heat exchanger
  - `ANAMHTEX`: Name of HCO(s) that represent the heat exchanger
  - `HTEXPAR1`: **Geometry parameter**
    - – For plate heat exchangers: chevron angle

- By assigning an HCO a specific HTEX type,
  - connected TFOs (primary and secondary) will be automatically determined
  - dedicated correlations for pressure loss and heat transfer coefficient will be automatically applied
  - alternative HTC models can optionally be used via PW `HTCCORR`

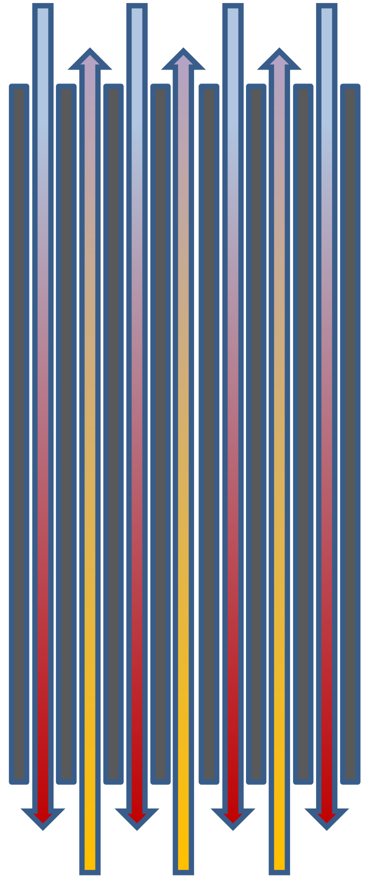
```
@     STEAM GENERATOR MODEL DATA
@     +++++++++++++++++++++++++
@
C---- STEAMGEN
@
K---- HXPLATE
@
@   IQP0     ISR0     QHE0    FPSTG
    0        1        0.0     %FPARHPLA%
@
@  ANAMS(K) SOS(I)            QSHE(I)
   'PLATE'  0.000             1.0
   'PLATE'  0.519             1.0
@
----- HTEXDEF
@  IHTEXTYP  ANAMHTEX  HTEXPAR1
   1         'PLATE'   %ANGLE%
```

Plate Heat Exchanger – Modeling Approach

Channel nodalization



Base geometry: 1 channel

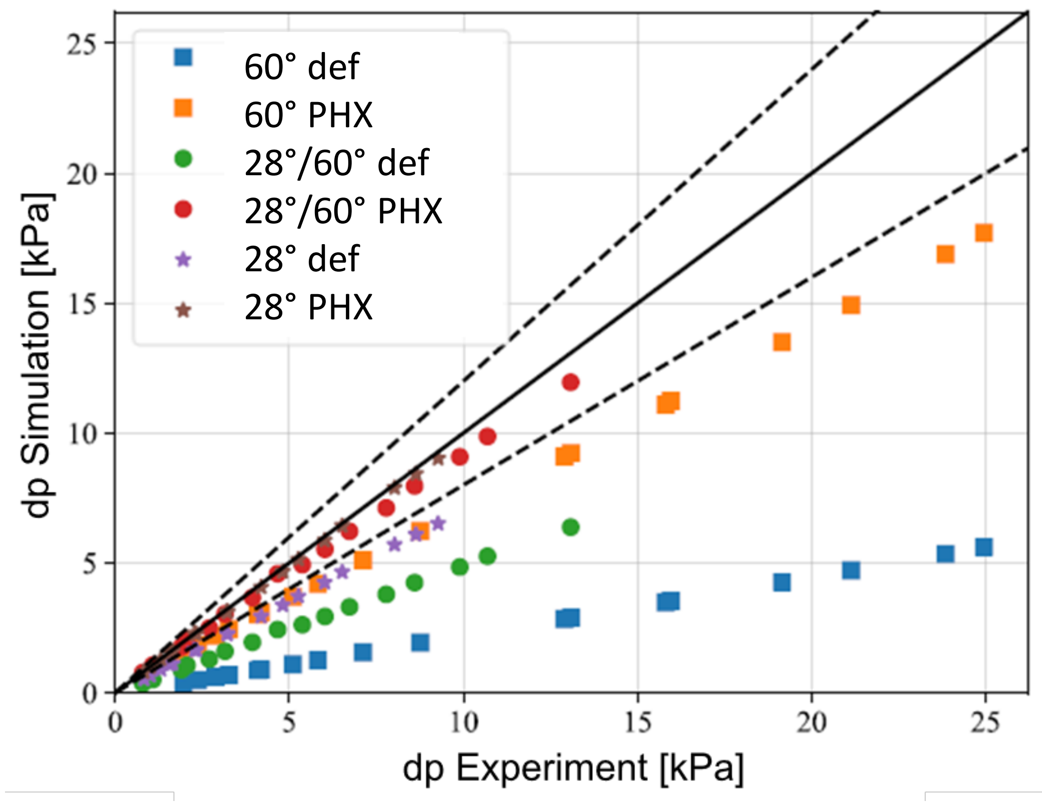


→ Plate: FPARH = FPARO_1 + FPARO_2 - 1

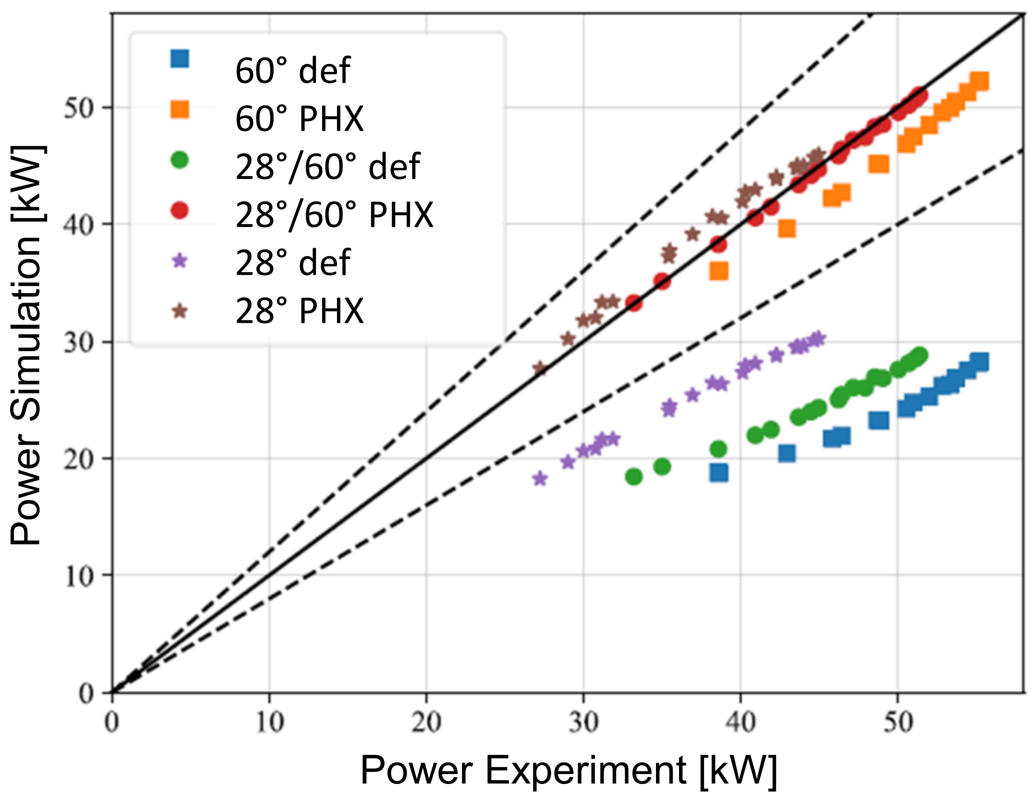
Model validation of single-phase correlations

- Johannesburg-Experiment[1] with stationary conditions using different chevron angles (working fluid: water)
- Significantly improved agreement with new correlations (PHX)

Pressure loss



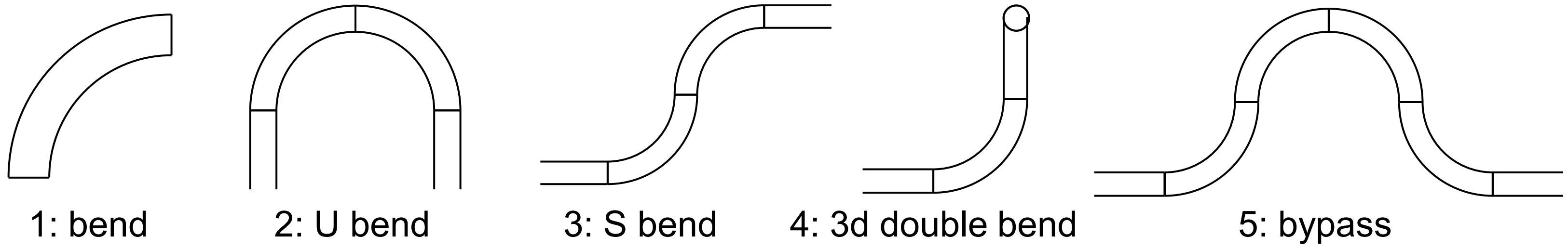
Heat exchanger power

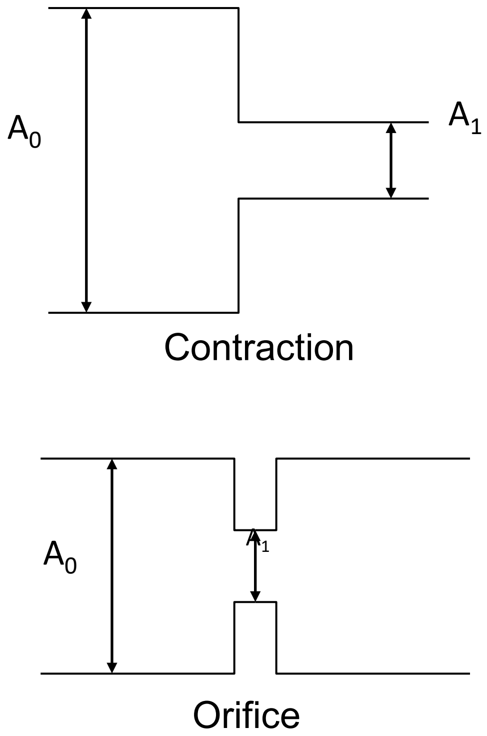


[1] *Huang, J.: Performance Analysis of Plate heat Exchangers used as Refrigerant Evaporators. University of the Witwatersrand: Johannesburg, August 2010*

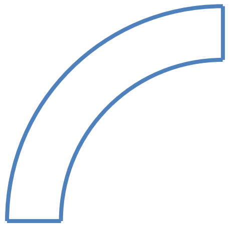
Reynolds-Number Dependent Form Losses

- **Motivation**: More accurate modelling of local form losses
  - **Start-up behavior** of (passive safety) systems
- New option to specify form loss coefficients **ζ dependent on Reynolds number** (instead of constant values)
  - Tabulated data can be provided by the user
  - Dedicated correlations available for several component types





Form Loss Definition under New CW FORMLOSS



90° bend

```
C----  FORMLOSS
K----  FL1
@        IFRMLTYP          ZETA0
         2                 0.50
@
@        RADIUS     ANGLE    BTYPE
         2.0        90.0     1
```

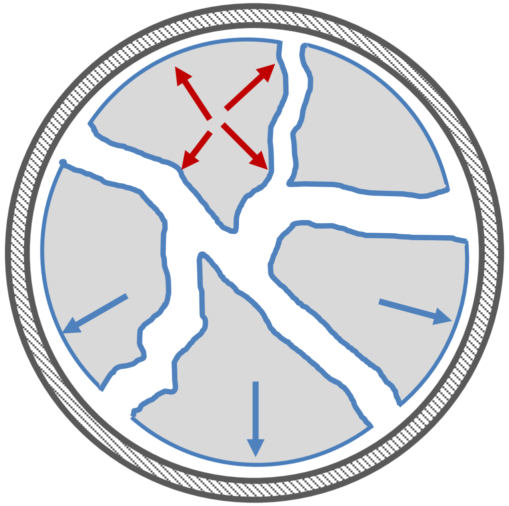
- IFRMLTYP: Defines the type of form loss
  - = 1: Tabulated values (CW TABLES)
  - = 2: Bend
  - = 3: Sudden contraction
  - = 4: Orifice
- Parameters, depending on IFRMLTYP

- For TFOs under PW FRICTION:
  - Like for constant values, the Re-dependent form loss must be assigned for each flow direction individually
  - Constant and Re-dependent form losses can be combined
  - The same form loss keyword can be assigned to an arbitrary number of junctions.

```
K----  P1-HL
 .  .  .  .  .
-----  FRICTION
@   ITPMO        ALAMO        ROUO
    2            0.02         1.D-5
@   SF0          SDFJ0        ZFFJ0        ZFBJ0
    0.           0.0          5.0          1.5
    5.0          0.0          FL1          FL1
    9.190        0.0          FL2          0.
    9.197        0.0          3.0          1.5
```

Improved Fuel Rod Model – Overview *

- **Motivation: Improved (best-estimate) prediction of DBA**
  - Former implementation could yield unrealistic (often too conservative) results for clad temperature
  - Simplified models with regard to gap size and gap conductivity
- Fuel rod model was improved through implementation of several new models:
  - **Prediction of fuel radial relocation, densification, and swelling effects**
  - **Evaluation of clad mechanical strain effects**
  - **Enhanced gas gap conductivity modeling**
  - Goal: Better predicting gap conductivity & size



Fuel swelling and relocation

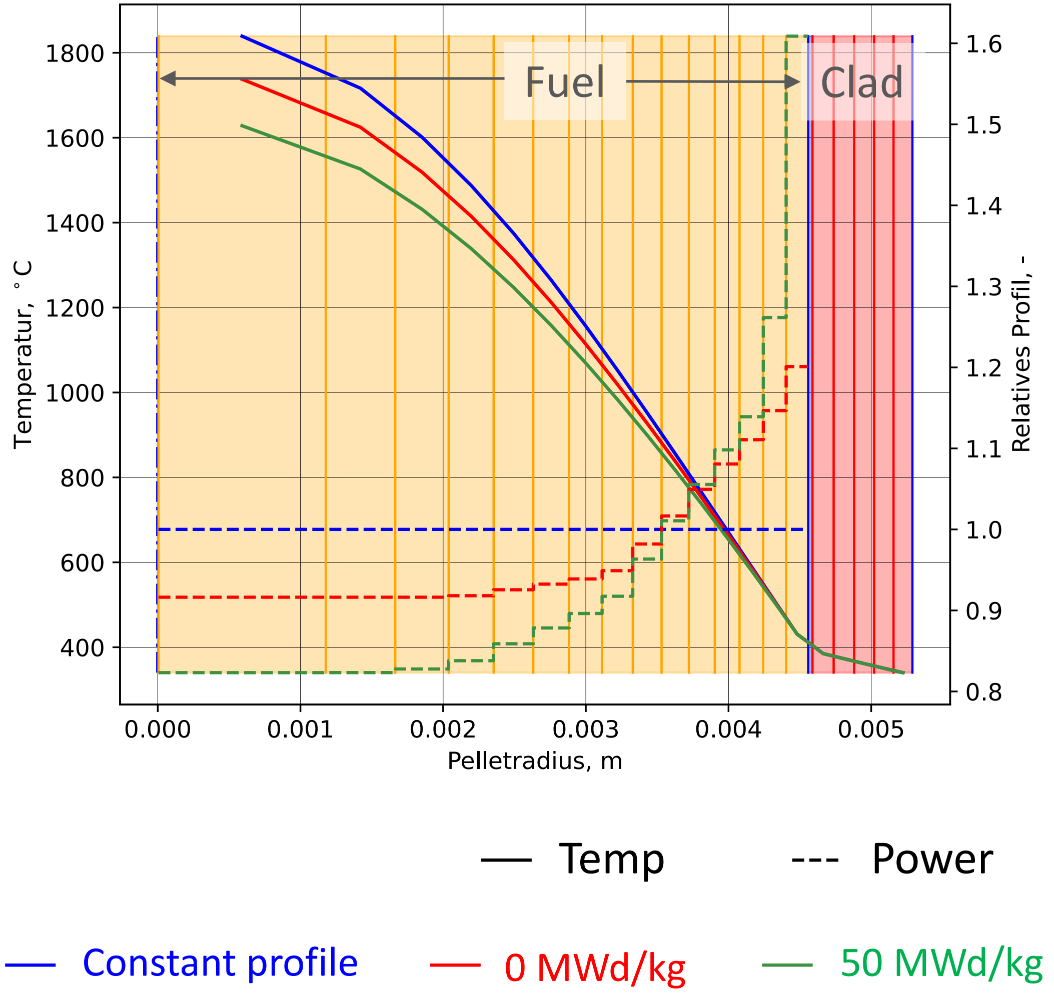
** Details see separate presentation by Anthony di Nora*

Simulation of rod radial power distribution via user-defined profile

- Allows for the modeling of more realistic rod radial power profile (varying, e.g., with burnup)
- Local relative power vs. relative radial coordinate required
  - i.e., profile abscissas between 0 & 1
  - profile ordinates > 0, internally normalized to 1.0

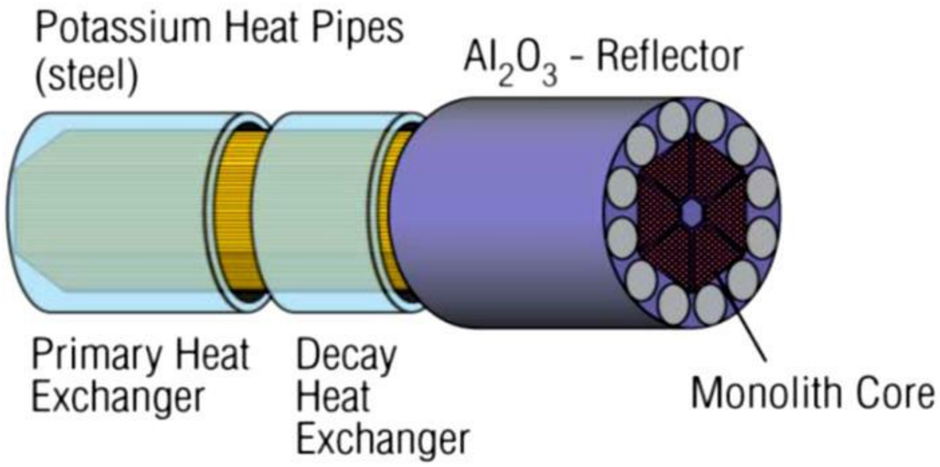
```
----- RADPOW
@       RRP0         RRPWR
        0.00000      0.83000
        0.47059      0.84000
        0.70588      0.92000
        0.94118      1.18000
        1.00000      1.80000
```

- Applied to the zone selected for the rod power generation (input parameter `IPOWM0`):
  - Planar, cylindrical, spherical geometries
  - Geometry factors are calculated internally



New Working Fluid Properties and NC Gas Components*

- **New Working Fluid Potassium**
  - **High-temperature heat pipes** of advanced Micro Modular Reactors utilise K or Na



J. W. Sterbentz et al.: Preliminary Assessment of Two Alternative Core Design Concepts for the Special Purpose Reactor. Idaho National Laboratory (INL), INL/EXT-17-43212 Revision 1, 2018

- **Updated Sodium Properties**
  - Correlation for η and λ of the vapour (constant before)
  - → Correlations for all Na properties

- **Further working fluids via coupling interface** available
  - Name `AFLUID` under CW `WORKFLUID`: **`EXTERNAL`**
    - Can be used for coupling to e.g. **CoolProp library** (http://www.coolprop.org/)
    - Config file to provide further settings required by CoolProp

- Properties for **additional NC gas components** implemented: **`XENON`** and **`KRYPTON`**

* *Details see separate presentation by Daniel Eckert*

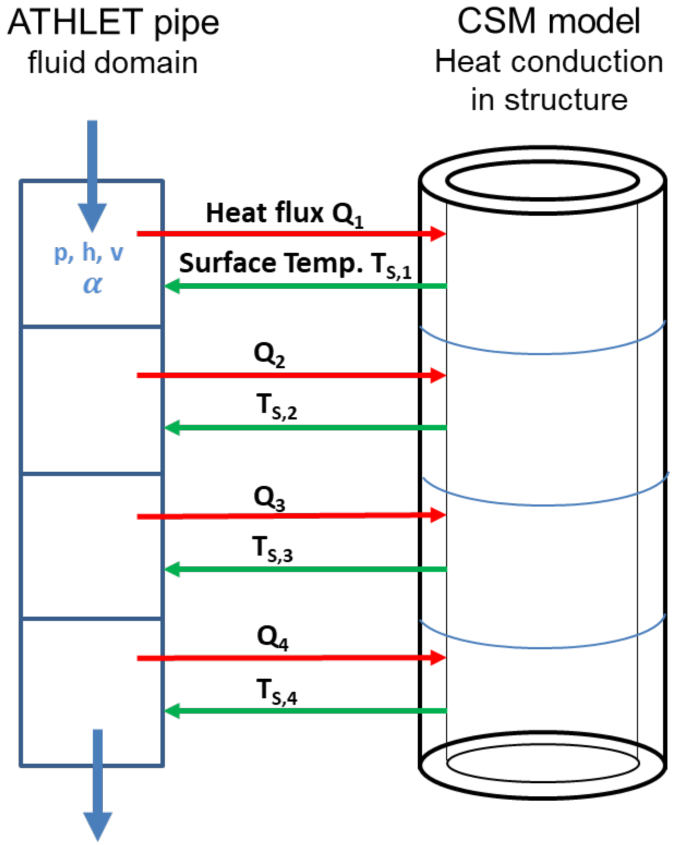
Gas Mixture Initialization: Input under CW **MULTICOMP**

- **New**: Initialization of NC gas mixtures
  - **Arbitrary mixture** of available NC gases
  - In single TFOs or complete TFD-systems
    - To initialize all TFOs of a TFD-system: ANAMO = “TFDSYS_<system-name>”
  - PW INITGAS
    - Defines first gas component and total gas volume fraction XQVMCI
  - **New PW INITXVMC**
    - Allows to initialize the mass ratio XVMCI of the second, third etc. gas component to the total gas mass

```
C----  MULTICOMP
@      NMCSYS      AMCSYS
       1           1
@      MCVN        AGAS
       2           NITROGEN     ARGON
@      MCLN        ALIQ
       0
@
-----  INITGAS
@      ANAMO        AGASO        XQVMCI
       GM_V1        NITROGEN      1.0
       GM_V1HC      NITROGEN      1.0
@
-----  INITXVNC
@      ANAMO        AGASO        XVMCI
       GM_V1        ARGON         0.01
       GM_V1HC      ARGON         0.01
```

Further Model Improvements in ATHLET 3.4

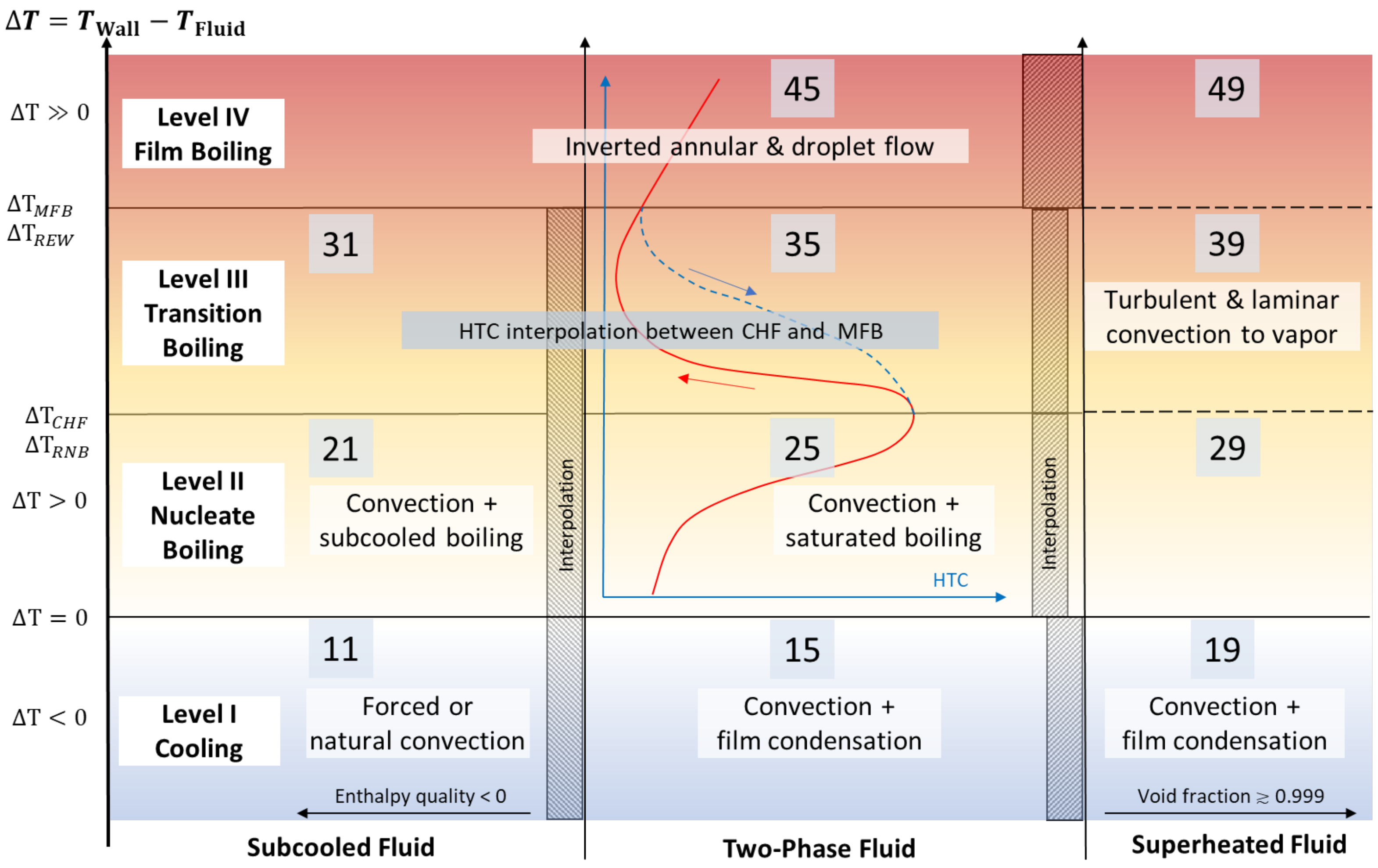
- New correlations for **Austenitic and Ferritic steels oxidation** (CW `HEATCOND`, PW `ZROXIDAT`)
- **Updated T-Model**: applicable with 2M-model, considers pressure drop/increase in 2M main pipe
- **New CHF correlation proposed by Song et al.**[1]
  - Mainly developed for high pressure conditions: $p > 0.7\ p_{crit}$
  - Can be activated by input parameters `ICHF1/6` = 13 (see CW `HEATCOND`, PW `CHFREWET`)
- **New interfaces to external models**
  - Coupling Interface to 3D-NK code FENNECS
  - **PreCICE adapter for coupling of ATHLET with other codes**
    - E.g. for coupling with 3D CSM solver CALCULIX



[1] *Song, M., Liu, X., Cheng, X.: Prediction of critical heat flux (CHF) for the high-pressure region in uniformly heated vertical round tubes. Annals of Nuclear Energy, Bd. 158*

Extended MHTCEXT Plug-in for User-provided HTC Correlation

- MHTCEXT plug-in comprises a set of interfaces for various heat transfer regimes and working fluids
- Extensions:
  - **Interface for film-boiling** (Mode 45)
  - **SC water**: updated parameter list: bulk viscosity, specific heat capacity and heat conductivity (Mode 21, 25)
  - **Convective heat transfer** interface usable **for any working fluid** (Mode 11, 15, 21, 25)



Extended Input Checks

- The **basic syntax for all CW is checked**. In particular it is checked:
  - If only legal CW are used, and only (sub-/pseudo-) keywords allowed for a CW are present
    - – Under CW `OBJECT`, legal PW are identified based on `ITYPO`
  - If all PW are input strictly in the order they are mentioned in the Input Data Description
  - Checks apply to ATHLET-CD CWs as well

- In most CW all **inputs are checked if they correspond to valid options**. Error messages explain the problem.
  - For input blocks with a fixed number of cards, it is **checked if spurious input is present**
  - Strings with more than 10 characters lead to an error, except where longer strings are allowed

- **Note: Most error print outputs come with the information on the questionable input deck line**

Input and Output Data Changes

- Optionally, SWs can be introduced
  - under CW `PARAMETERS` to organize parameters and to easily (de-)activate complete sets of parameters
  - under CW `HEATCOND` to structure the list of HCOs
  - **check the Program Updates Manual for further changes** of input and output data!

- **Input data deviations from default values are printed to the log-file***

- **Additional data in the hdf-5 file**: TFO/HCO geometry data; units for all quantities **

- In order to harmonize the key file and the requirements of hdf-5 data, **all „/“ in ATHLET and ATHLET/CD output variables have been replaced by „_“**
  - E.g. HECU quantities TT_, TTRISO_, QAXH_

- Where there were leading „0“ for the quantity, now the actual number will be output left-aligned **without leading zeros**: E.g. RMVMC_1 instead of RMVMC/001

** Details see separate presentation by Andreas Wielenberg*
*** Deails in presentation by Markus Junk*

Conclusions

- **Numerous new and improved models included in ATHLET 3.4.0**
  - Heat transfer and pressure loss correlations for **compact heat exchangers** in SMRs
  - Improved consideration of form losses
  - Widely updated **fuel rod model** for DBA analyses
  - **New two-phase working fluids** and NC gas components
  - Divers model updates, e.g. T-junction model, oxidation model

- **User support by additional error checks and expanded output data**
  - **Extensive input data checks** for the complete ATHLET and ATHLET-CD input deck
  - Information on **input data deviations from default values**
  - Various new input data options
  - **Expanded output data in hdf-5 file and in print output** for further analyses

The development and validation of AC²/ATHLET are supported by the German Federal Ministry for the Environment, Nature Conservation, Nuclear Safety and Consumer Protection.

Supported by:

Federal Ministry
for the Environment, Nature Conservation,
Nuclear Safety and Consumer Protection

based on a decision of
the German Bundestag