New Models and Features in ATHLET 3.5

Philipp Schöffel, GRS

AC² User Meeting, GRS Köln, 18.11.2025

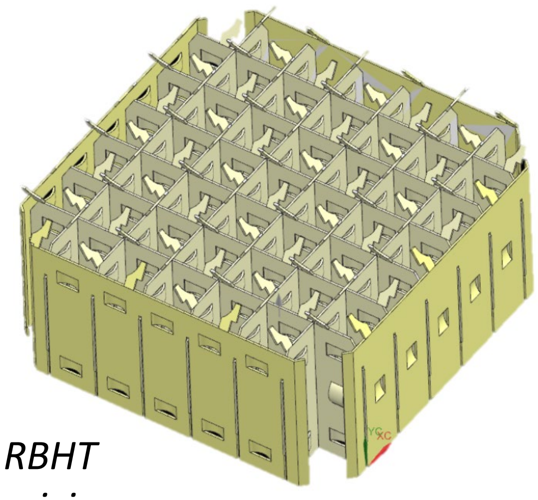
Content

- **New and Updated Models in ATHLET 3.5**
  - New models for **structures and internals**
    - Spacer grid modelling
    - Geometry, materials and heat conduction in HCOs
  - Extended **Flow Regime Maps and Friction Loss Models**
  - Component Model Updates: **Heat Pipe, Critical Discharge**
- **Input, Output and Postprocessing**
  - 3D TFO and HCO data
  - New Input Options and Output Data
- **Summary**

Modelling of Rod Bundles with Spacer Grids

Objective: Capture spacer grid effects on **TH behavior during core uncovery**

- **Convective heat transfer enhancement** downstream the spacer grid
- Increase of interfacial area and interfacial transfers due to **droplet breakup**



RBHT mixing vane spacer grid

Previous ATHLET spacer grid model only considered impact on CHF

- Applicable with **Groeneveld LUT**

$$q_{\text{CHF,spacer}} = \left[1 + A\exp\left(\frac{-B\,L_S}{D_H}\right)\right] q_{\text{LUT}}$$

- Requires provision of input data under
  - PW SPACER (HECU) defining positions of spacer grids
  - PW FRICTION (TFD) with mandatory zeta value for each spacer grid junction

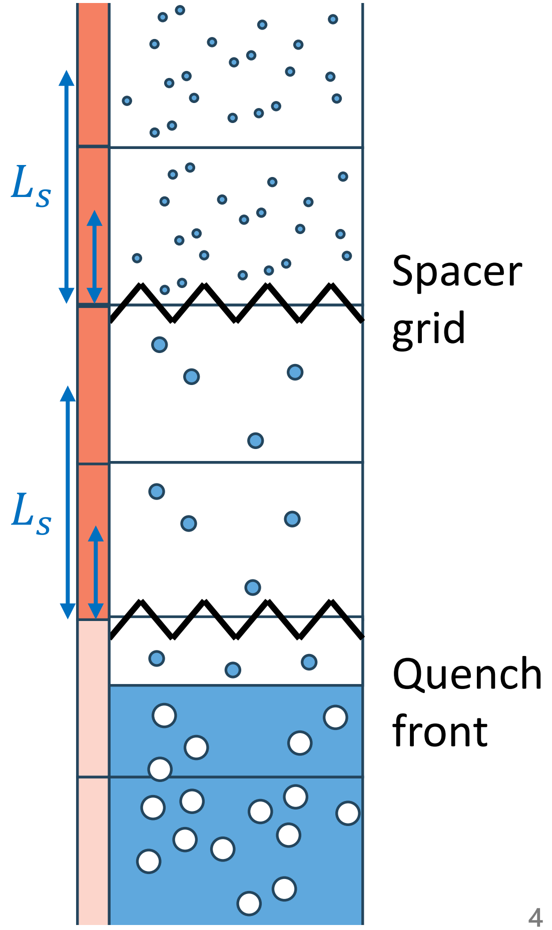
```
C---- HEATCOND
K---- HEATRIN
. . .
----- SPACER
@ SHSPAC0 (1...N)
  0.102   0.690   1.212 . . .
```

Extended Spacer Grid Model

- Turbulence-induced **convective heat transfer enhancement** downstream the spacer grid
  - Model options depend on **blockage ratio ε or friction loss K_g**
  - Yao: $Nu_{spacer} = \left(1 + 5.55\varepsilon^2 e^{-0.13(L_s/d_h)}\right) \cdot Nu_0$
  - Holloway: $Nu_{spacer} = \left[1 + \left(0.8K_g - 0.4\right)e^{-0.25(L_s/d_h)}\right] \cdot Nu_0$
- Increase of interfacial area due to **droplet breakup**
  - **Reduced droplet Sauter mean diameter** downstream the grid, considered by evaporation model

$$\frac{d_{32}}{d_0} = 6.167 \cdot We^{-0.53}$$

  - Applied for dispersed flow regime
  - Considers quench front progression (if model is active)

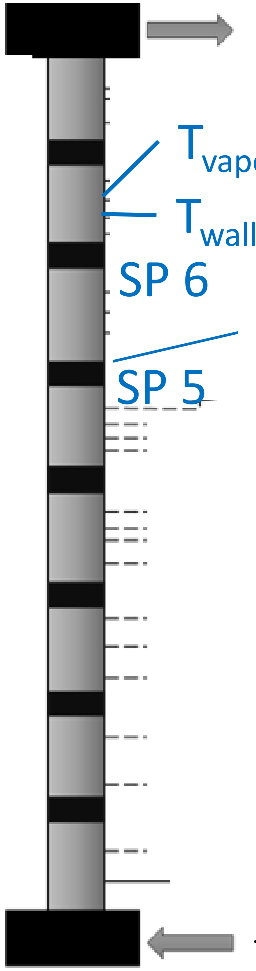


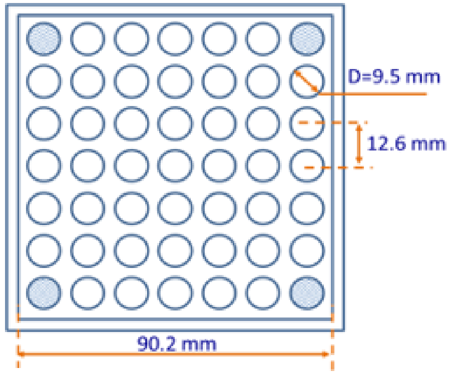
Validation against RBHT Experiment

OECD RBHT project

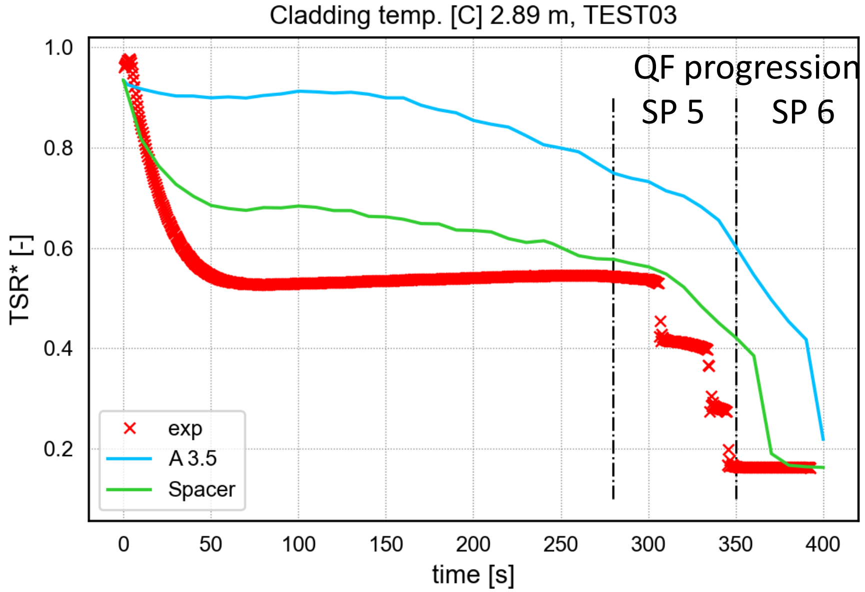
- Reflooding tests
- Pressure: 1 to 4 bar
- Subcooling: 3 to 80 K

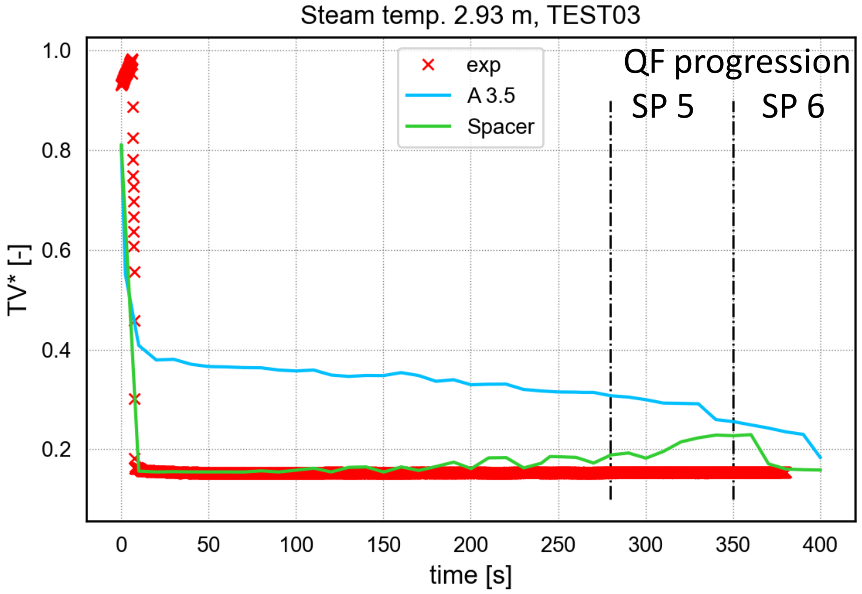
Cladding precooling downstream of the spacer grid





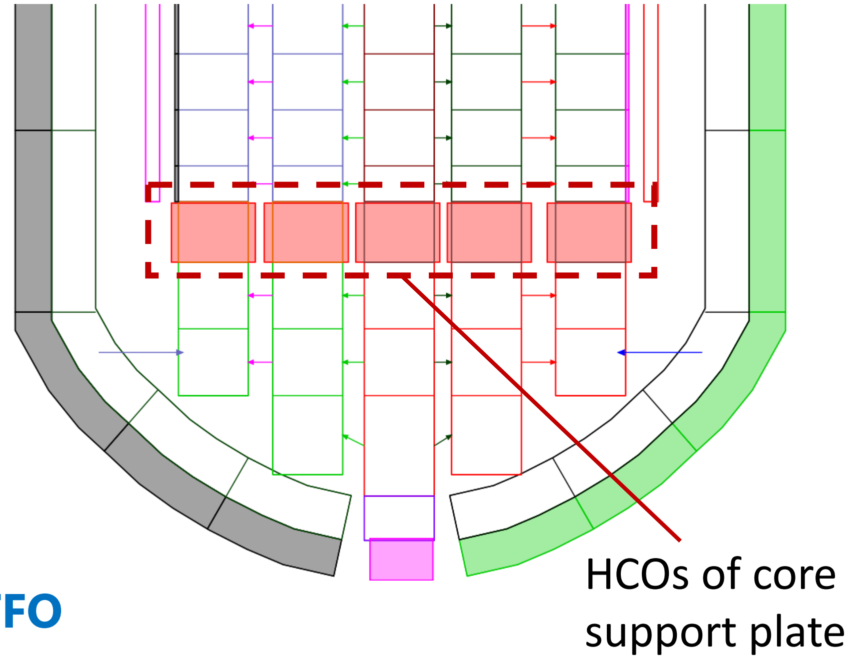
S. Bajorek and F.-B. Cheung: Rod Bundle Heat Transfer Thermal-Hydraulic Program; Nuclear Technology 205, 2019



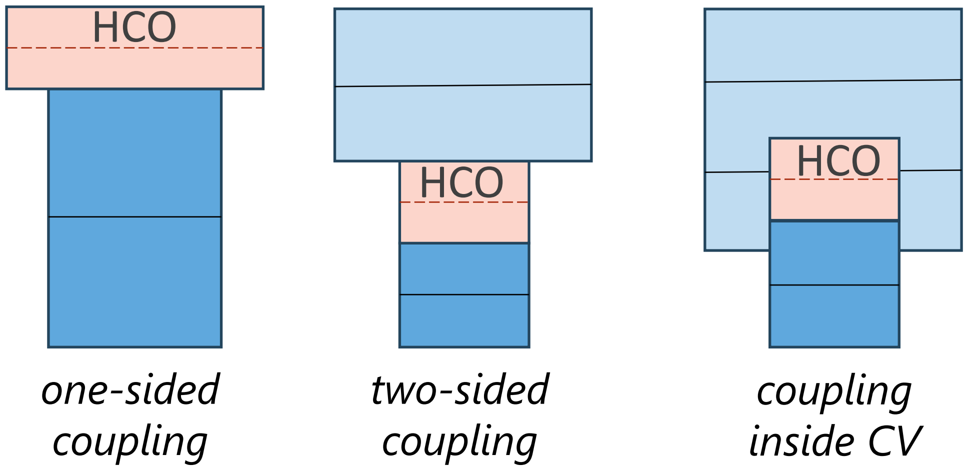


Simulation of Horizontal Structures

- Vessels or pools represented by vertically oriented TFOs
  - Up to now, coupling of an HCO only along axial direction of the corresponding TFO
  - **Limited accuracy** to model e.g. vessel lid, pool bottom, or a tie plate
  - **Need to couple an HCO orthogonally to a vertical TFO**

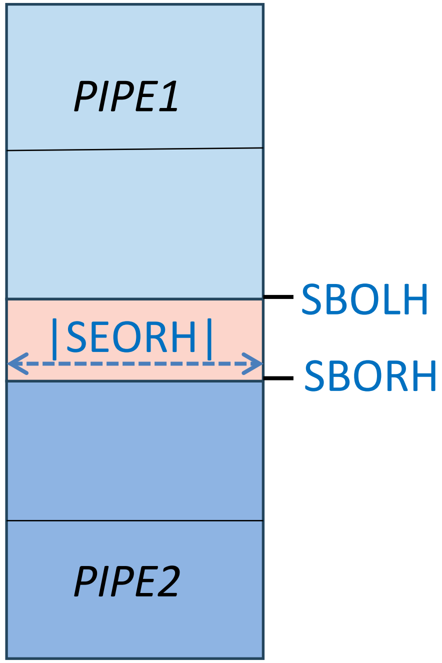


- **New HCO type "horizontal plate"** introduced
  - enables to couple a strictly horizontal HCO orthogonally to a (strictly vertical) CV
  - always consists of a single HCV



Application of Horizontal Plate

```
K---- HORPLATE
@ AOLH  SBOLH SEOLH AORH  SBORH SEORH
  PIPE1    0.   -0.2 PIPE2    5.   -0.2
@ . . . IGEO0 ...
  . . .     0 ...
----- GEOMETRY
...
@ SG0  Z0  DI0  DS10 GAP10 ...
  0.   1.3 0.15 0.05 0.    ...
  0.2  1.3 0.15 0.05 0.    ...
```



- **By convention, the left side is the upper side**, the right side the lower side
- Coupling location inside the TFO is determined by SBOLH resp. SBORH
- A negative input value for SEOLH or SEORH indicates horizontal coupling. Its absolute value must be equal the length of the plate.

- Horizontal plate during application:
  - **Churchill correlation** for natural convection heat transfer at top and bottom side:

$$Nu = c \cdot \left[Ra \cdot \left[1 + \left(\frac{d}{Pr} \right)^{a} \right]^{-1/a} \right]^{b}$$

  - No specific correlations in other heat transfer regimes

New Options for Structure Materials

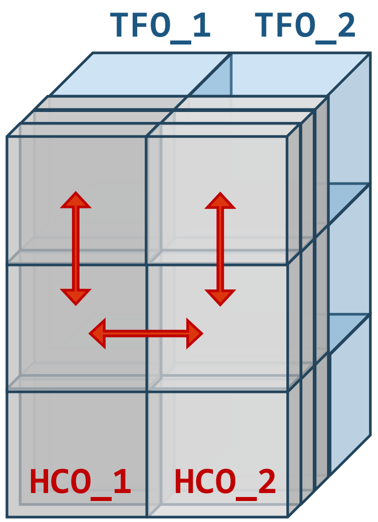
- HCOs may optionally consist of **more than three material zones**
  - **Input parameter `NADDMZ`:** number of additional zones
  - Extension of further PWs where relevant, e.g. GEOMETRY, HTCDEF, MATPROP

```
K---- H_BOILER   @ split into 6 material zones
@  AOLH         SBOLH  SEOLH   AORH          SBORH  SEORH
   ADIABAT      0.     0.      BOILER        0.02   0.07
@  NIHC0 N10 N20 N30 IGEO0 ICOMP0 ACOMP0   ICHF0 NADDMZ
   1      10  2   2   5      0      DUMMY    2      3
@  N40  N50  N60
   2    2    2
@
----- GEOMETRY
. . .
----- HTCDEF
```

- Additional built-in materials available: **BORCARBIDE, INCONEL600, ALUMINA** (Al_2O_3)

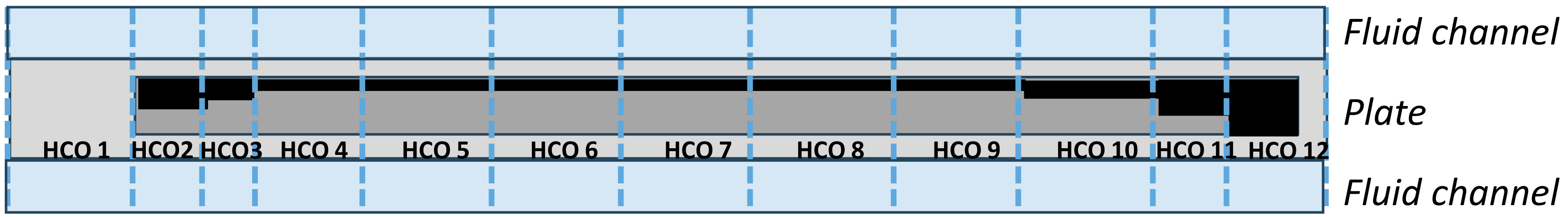
Simulation of 3D Heat Conduction in Structures

- **Motivation**: Detailed simulation of complex structural components
  - Usage of a 3D TFD network requires refining the HCO network
  - So far, HECU solved for a 1D or a pseudo-2D heat conduction equation
- **New CW `HCOCONNECT`** enables **3D heat conduction** by coupling of HCOs
  - Prerequisite: equal axial nodalization and equal number of layers
  - Alternative sparse matrix solver from PETSc package




```
C---- HCOCONNECT
@   IHCSYS
    4
K---- Group1
 .  .  .  .
@   AHCOLIST(1,…,n)
    HCO_1  HCO_2   ...
```

- **Application**: plate-type fuel elements in research reactor *

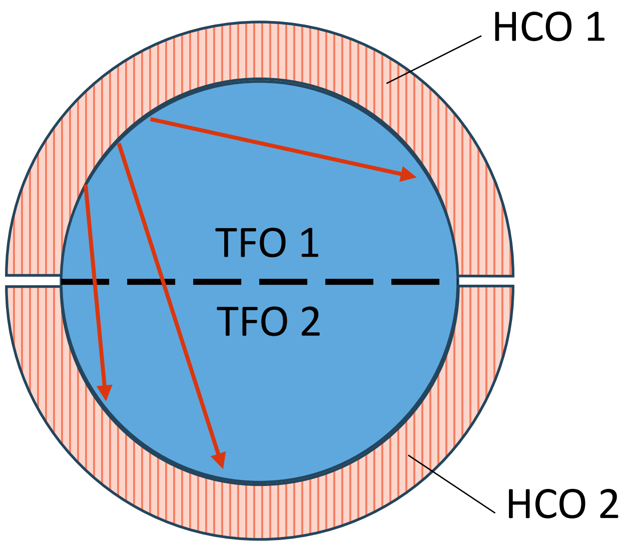


** See presentation by F. Weyermann*

Extended Thermal Radiation Model

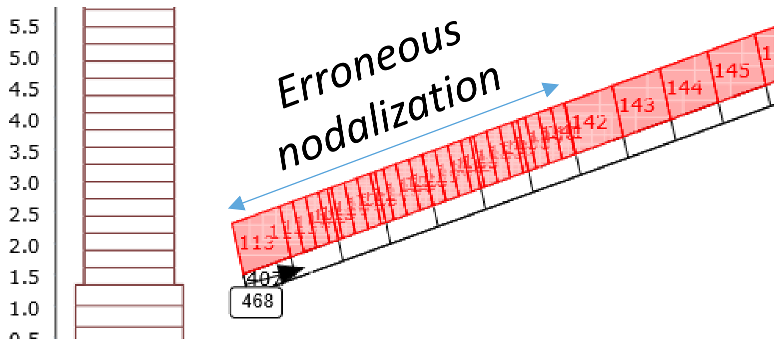
Thermal radiation between HCOs connected to *different* TFOs

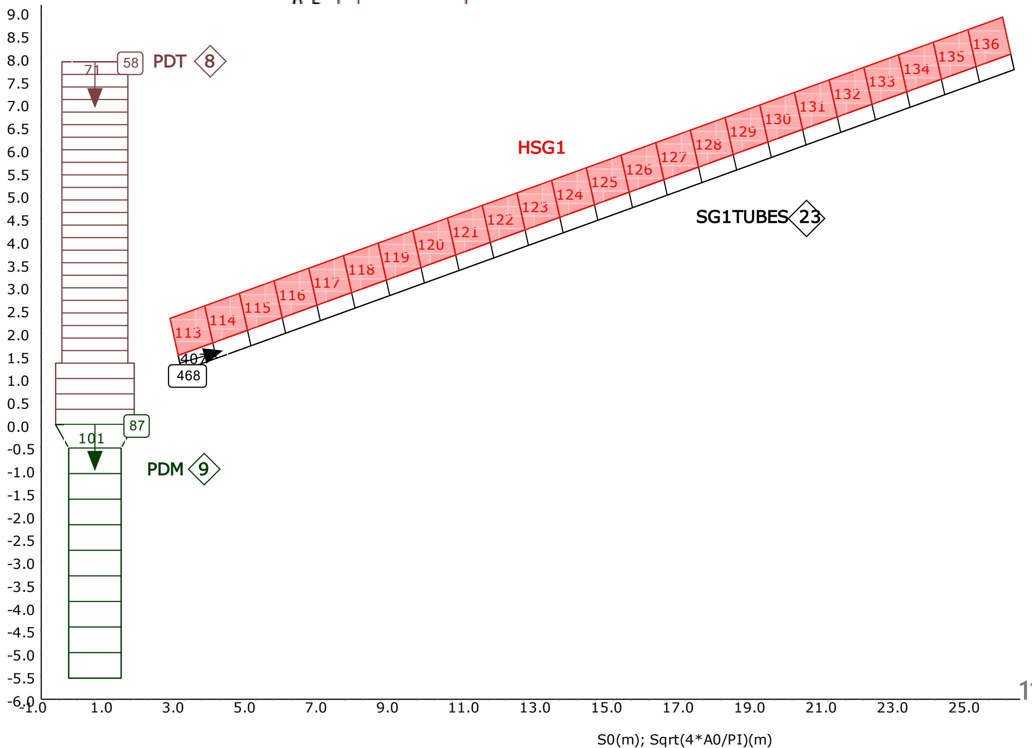
- Definition of radiation group under **new KW `FLEXRAD`**
- All grouped HCOs must have the same length
- Optional shape factor s for energy flux: $E = s \cdot \epsilon \cdot \sigma \cdot T^4$
- **Additional input check** to ensure reciprocity: $A_1 \cdot \varphi_{1\rightarrow 2} = A_2 \cdot \varphi_{2\rightarrow 1}$



Improvements of HECU Module for Helically Coiled HTEX

- Inside helical heat exchanger tube, **HTC calculation under film boiling conditions** uses Mc Eligot correlation (avoids program error)
- Improved automatic **HCO nodalization for non-congruent TFO/HCO**
  - Helical coil represented by inclined pipe
  - Erroneous HCO nodalization results caused program stop
    - Depending on orientation of inner and outer side TFOs
    - Work around: introduce numerous HCOs each consisting of one HCV
  - Improved program implementation provides HCO **nodalization that matches both adjacent TFOs**
  - **Increased user friendlyness**





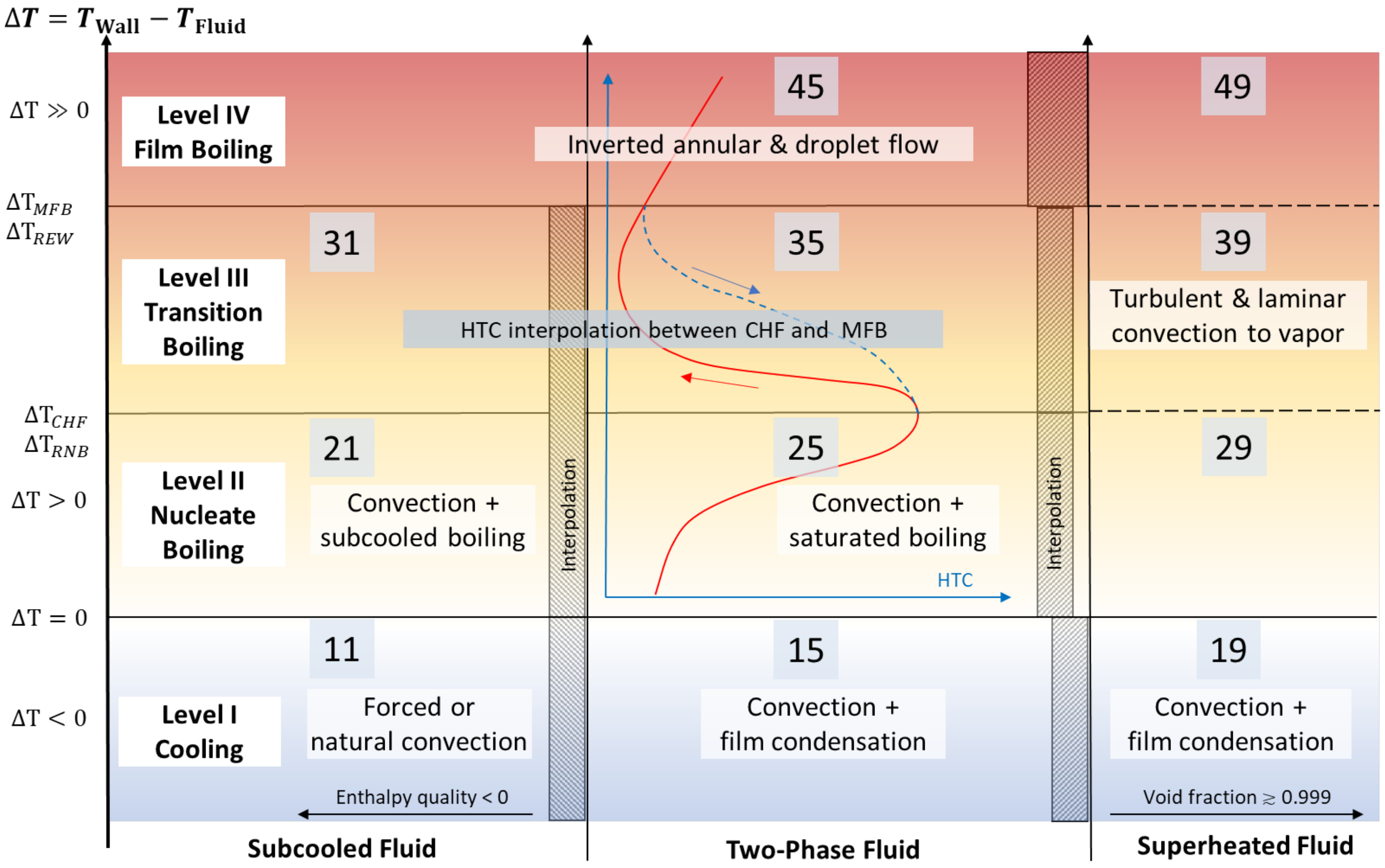
Extended Plug-ins for User-provided HTC and CHF Correlations

MHTCEXT plug-in

- Comprises set of interfaces for various heat transfer regimes and working fluids
- **New interface** for convective heat transfer to vapor in **DFFB regime (mode 49)**

Extended CHF plug-in

- Interface provides **access to TH quantities at core channel entry**
- **OMP-safe access to ATHLET global variables** via plug-in function *execute_c*

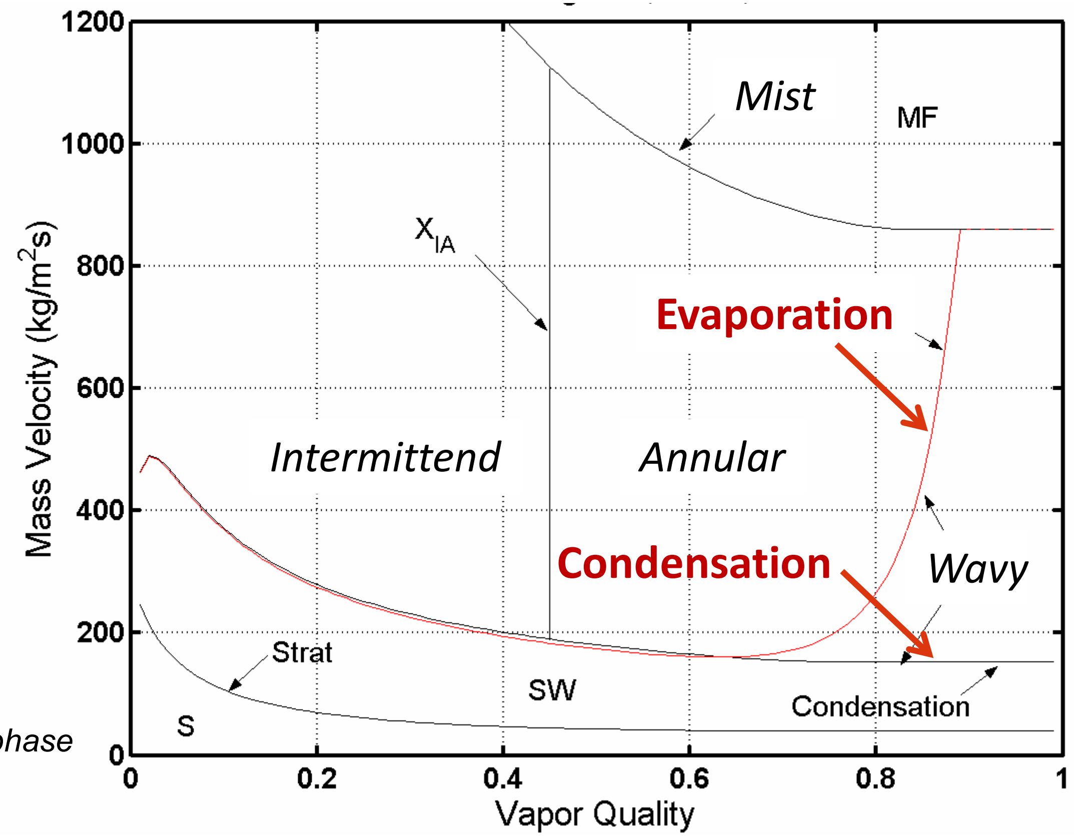


Unified and Extended Flow Regime Maps

- **Motivation**: Use of dedicated flow regime maps for both boiling as well as condensing flows
  - Centralized flow regime calculation (based on Taitel-Dukler) with **unified flow pattern map**
  - Unified calculation of the entrained liquid fraction
  - Output of current flow regime
- For **flows with wall condensation (passive systems)**
  - **Adjusted flow regime map** focusing on **horizontal annular flow**
- Steady transition between flow regime maps for

$$-1\,°\mathrm{C} \leq T_{\mathrm{wall}} - T_{\mathrm{sat}} \leq 0\,°C$$

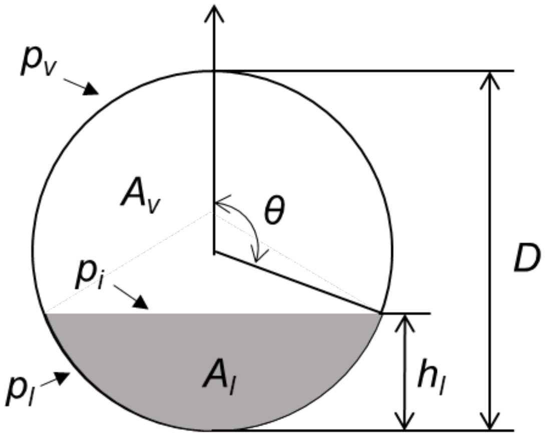
- Optional model, to be activated under CW MISCELLAN



* *Hajal, J. E., Thome, J. R., Cavallini, A.: Condensation in horizontal tubes, part 1: two-phase flow pattern map. International Journal of Heat and Mass Transfer, Bd. 46, Nr. 18, 2003.*

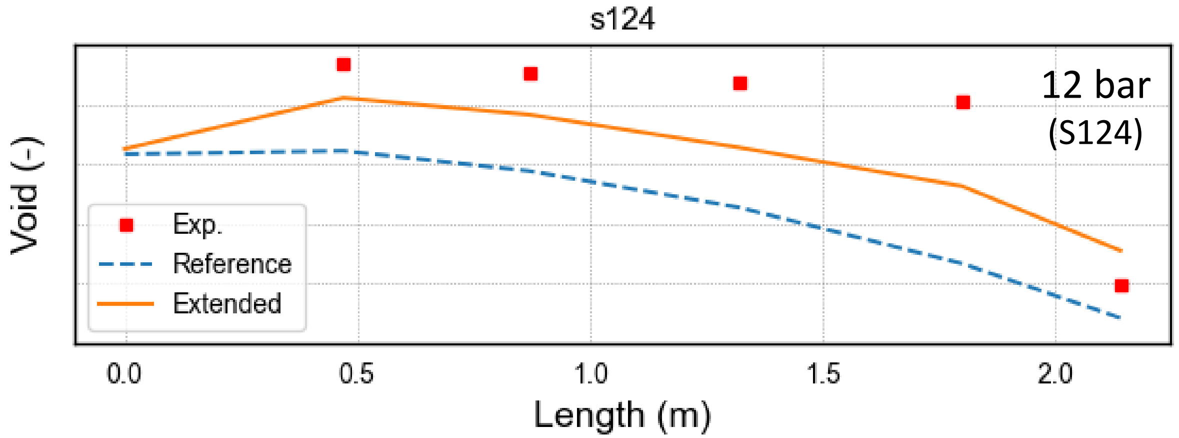
Closure Laws for Flow Regimes with Wall Condensation

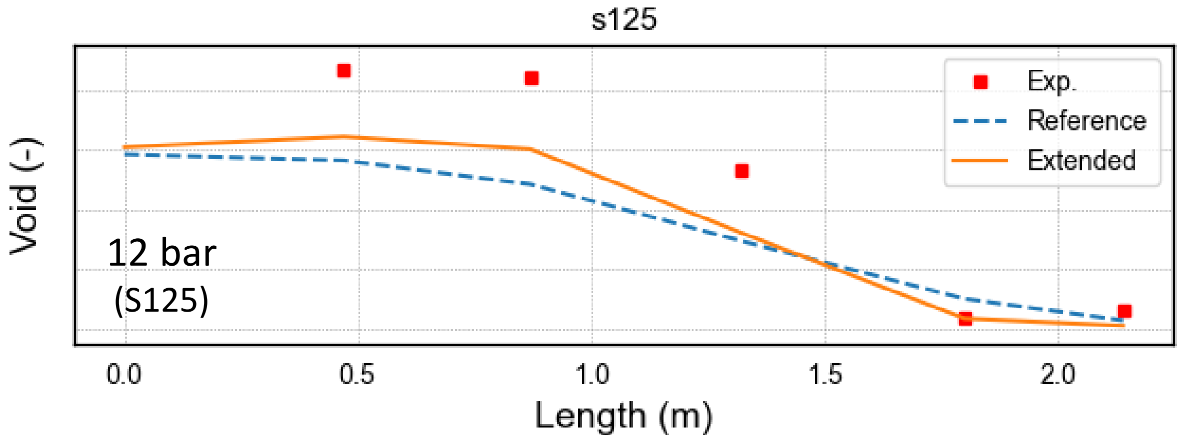
- Dedicated closure laws for **annular flow and stratified/stratified wavy flow**
- **Interfacial friction**
  - $C_{i,str} = \frac{1}{2}\rho_v\lambda_v\frac{4\sin\theta}{D_h\pi}$ (Taitel-Dukler)
  - $C_{i,\mathrm{wavy}} = \frac{1}{2}\rho_v\lambda_v\left(1+15\left(\frac{h_l}{D_h}\right)^{0.5}\left(\frac{j_v}{j_{v,crit}}-1\right)\right)\frac{4\ \sin\theta}{D_h\pi}$ (Andritsos-Hanratty)
  - $C_{i,\mathrm{ann}} = \frac{1}{2}\rho_v 0.005[1+75(1-\alpha)]\frac{4}{D_h}\sqrt{\alpha}$ (Wallis)
- **Wall friction** distribution to phases according to dry / wetted perimeter
  - Annular flow: wall friction completely assigned to liquid phase

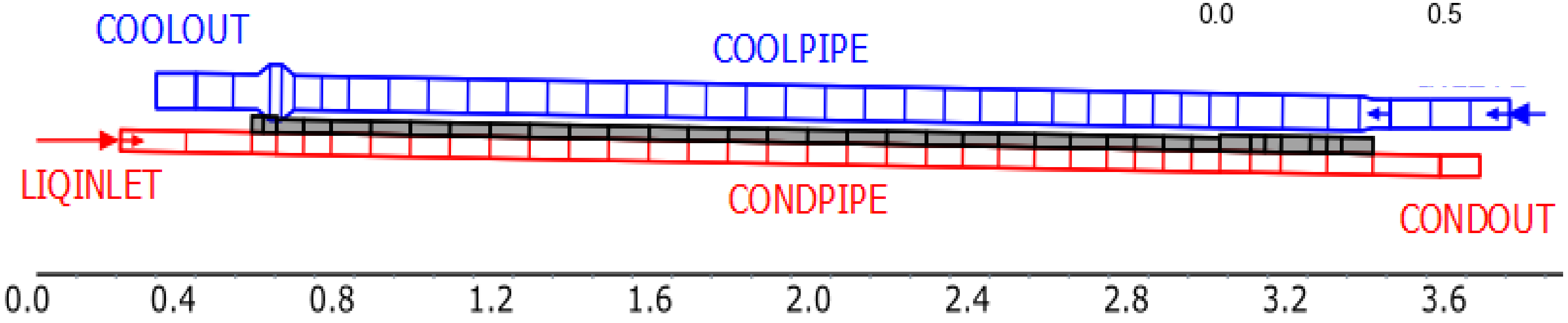


Validation of Flow Regime Map Module for Horizontal Pipe

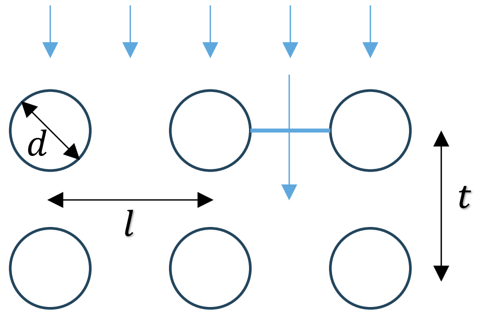
- **COSMEA experiment** with coaxial double pipe
- Slightly inclined pipe (L = 2.82 m, D = 43 mm)
- Condensation of steam in inner pipe
- On-going work related to
  - **Wall heat flow distribution** to phases
  - **Harmonization of wall condensation and bulk condensation models**

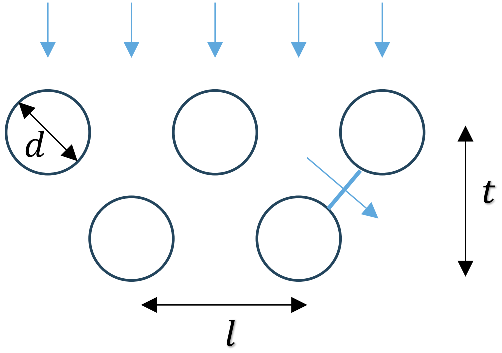






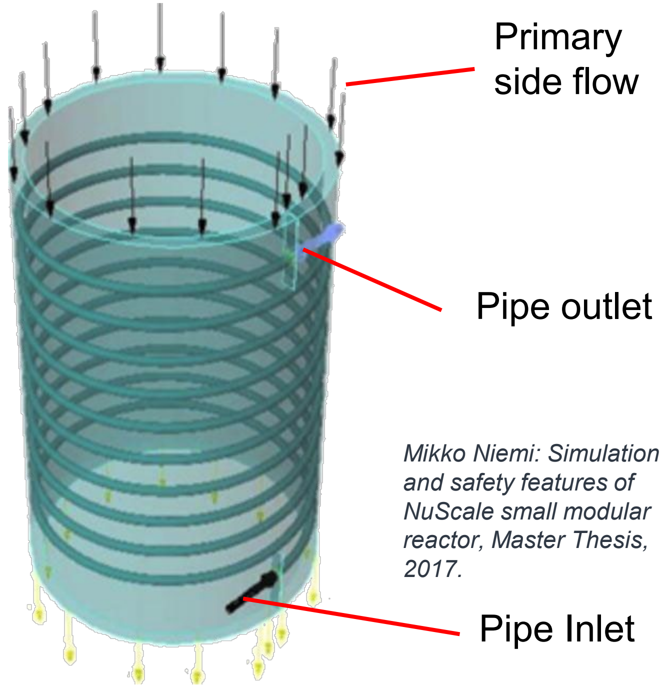
Friction Loss for Special Components





Cross flow in bundle (in-line or staggered arrangement)

- friction loss **ζ dependent on Reynolds number** $\zeta = \zeta_{\text{lam}} + \zeta_{\text{turb}} \cdot F(Re)$
- Dedicated correlation to be activated via CW `FORMLOSS`
- Automatically employed for helical heat exchanger (PW `HTEXDEF`)



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

For helical heat exchanger (inner side)

- Modified friction factor *: $\lambda_{\text{helix}} = \lambda_{\text{turb}} \left(Re \left(\frac{d_h}{d_{\text{coil}}} \right)^2 \right)^{1/20}$
- 2-phase flow with modified Martinelli-Nelson multiplier Φ_{tt}
- Development by RUB/J. Krieger **

** Nariai et al.: Friction pressure drop and heat transfer coefficient of two-phase flow in helically coiled tube once-through steam generator, J. Nucl. Sic. Technol. 19, 1982*

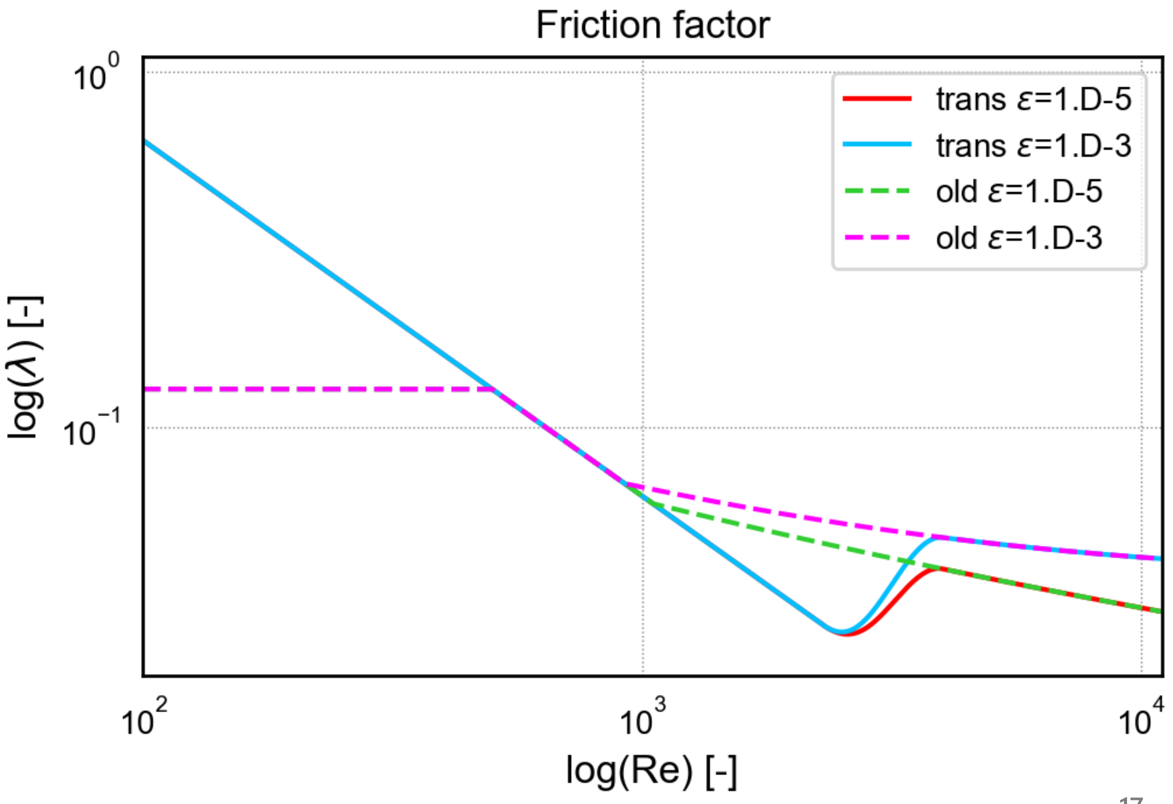
*** Krieger et al.: Simulation of the experiment OSU-002 regarding the behavior of a helically coiled steam generator using AC²-ATHLET, ICONE30, 2023*

Wall Friction in Laminar-turbulent Transition

Motivation: improved calculation of wall friction at **low Re-numbers** (IKE, M. Abd El Malek)

- **Start-up behavior of passive systems**
- So far, Darcy-Weisbach friction factor as maximum of Hagen-Poiseuille and Colebrook: $\lambda=\max(\lambda_{\text{lam}}, \lambda_{\text{turb}})$
- **Improved model with cosine-shape transition** between λ_{lam} and λ_{turb} for $2300 \le Re \le 4000$
  - For laminar flow: limitation of λ to $Re_L \ge 5$
  - Default model for pipe and annulus geometry
  - Input parameter **ITRNS** to select friction model
  - Adjustable Reynolds **interpolation range**

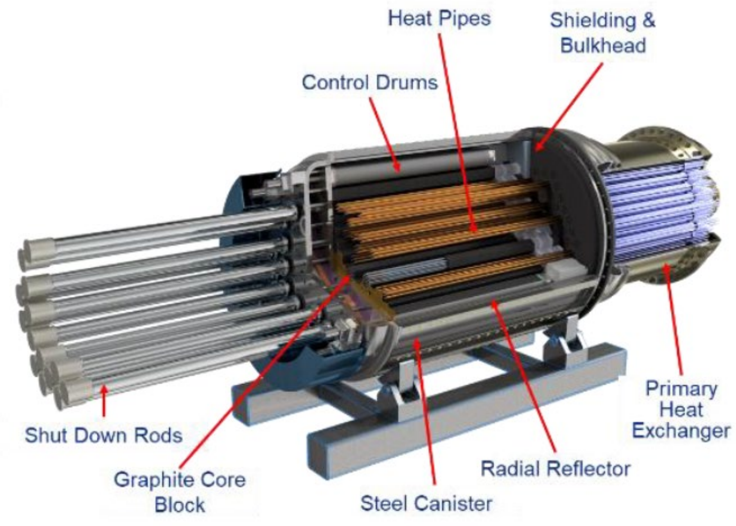
```
----- FRICTION
@     ITPMO   ALAMO   ROUO
      2       1.0     1.D-5
@
@     ITRNS   TRNS1   TRNS2
      1       2000.   3000.
```



New Feature: High-Temperature Heat Pipe Module

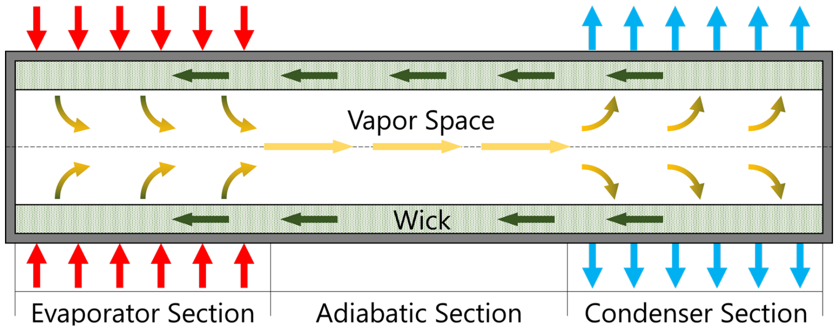
- **Liquid metal heat pipe-cooled MMR** (eVinci, SPR, …)
- Development of ATHLET for MMR safety analysis
- ATHLET Heat Pipe Module comes with **specific models** *
  - **Wick structure, capillary pumping, phase change, friction loss**
  - Covers **different wick types** and materials
  - Working fluids: Sodium, Potassium
  - Works with NC gases
  - For horizontal and vertical heat pipes

** Details in presentation by D. Eckert*



eVinci reactor system overview

Hong Xu, Yizhou Yan, Oriol Noguera Oliva, "CFD Thermal Analysis for Primary Heat Exchanger of eVinci^{TM} Nuclear Test Reactor", 21th International Topical Meeting on Nuclear Reactor Thermal Hydraulics, Busan, South Korea, August 31th - September 5th 2025



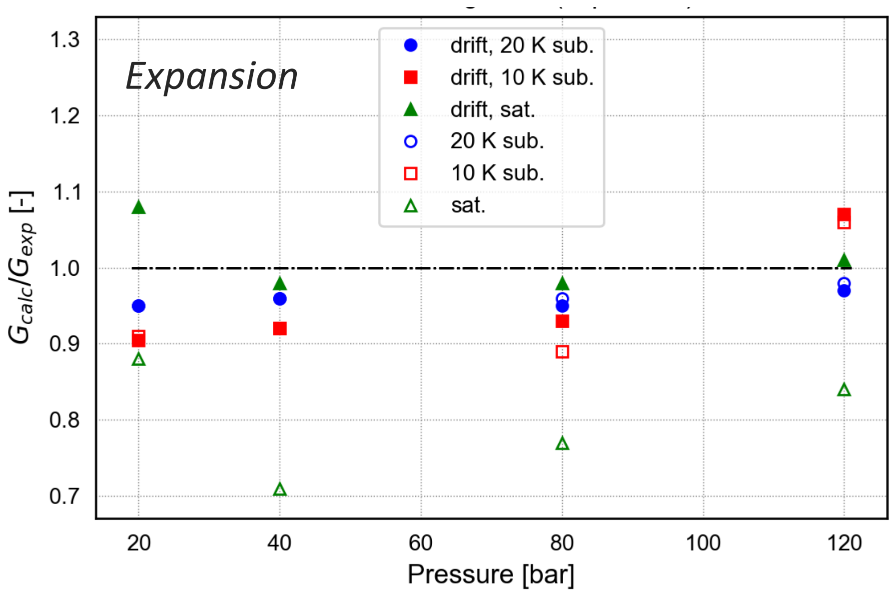
New Option for Critical Discharge Rate Calculation

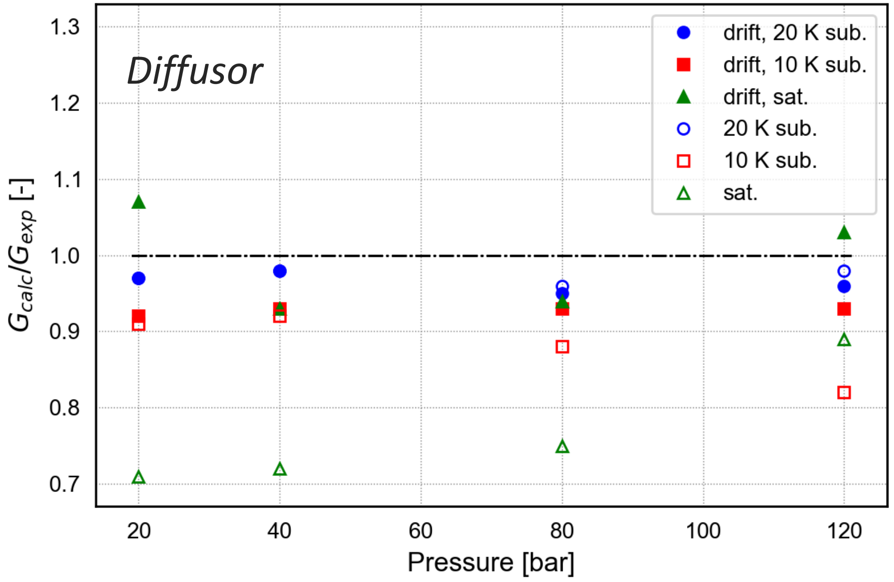
Critical discharge model CDR1D extended by optional **consideration of phase drift**

- 4-eq. system with phase slip

$$S = 1 + \frac{3}{2}\sqrt{3\alpha}(1-\alpha)\left(\left(\frac{\rho_l}{\rho_v}\right)^{1/3} - 1\right)$$

- Application of ATHLET standard evaporation model:
    - Input parameter **TURB defines bubble number density**
- Activated under CW DISCHARGE: IAUR=5
- Validation against Super Moby Dick experiment
    - 20 mm nozzle
    - Two different geometries investigated: Sudden expansion or diffusor
- Further model validation required



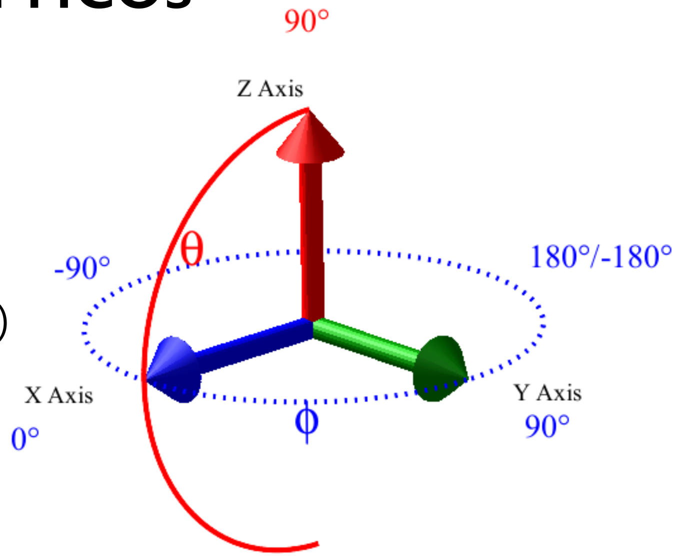


Integration of ATHLET-CD

- **Ongoing ATHLET-CD integration into ATHLET** makes several modules available *
  - 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)
  - Enables accident simulation without core degradation/until melting

** Details in presentation by L. Lovasz*

New Input and Output Options: 3D Data for TFOs and HCOs



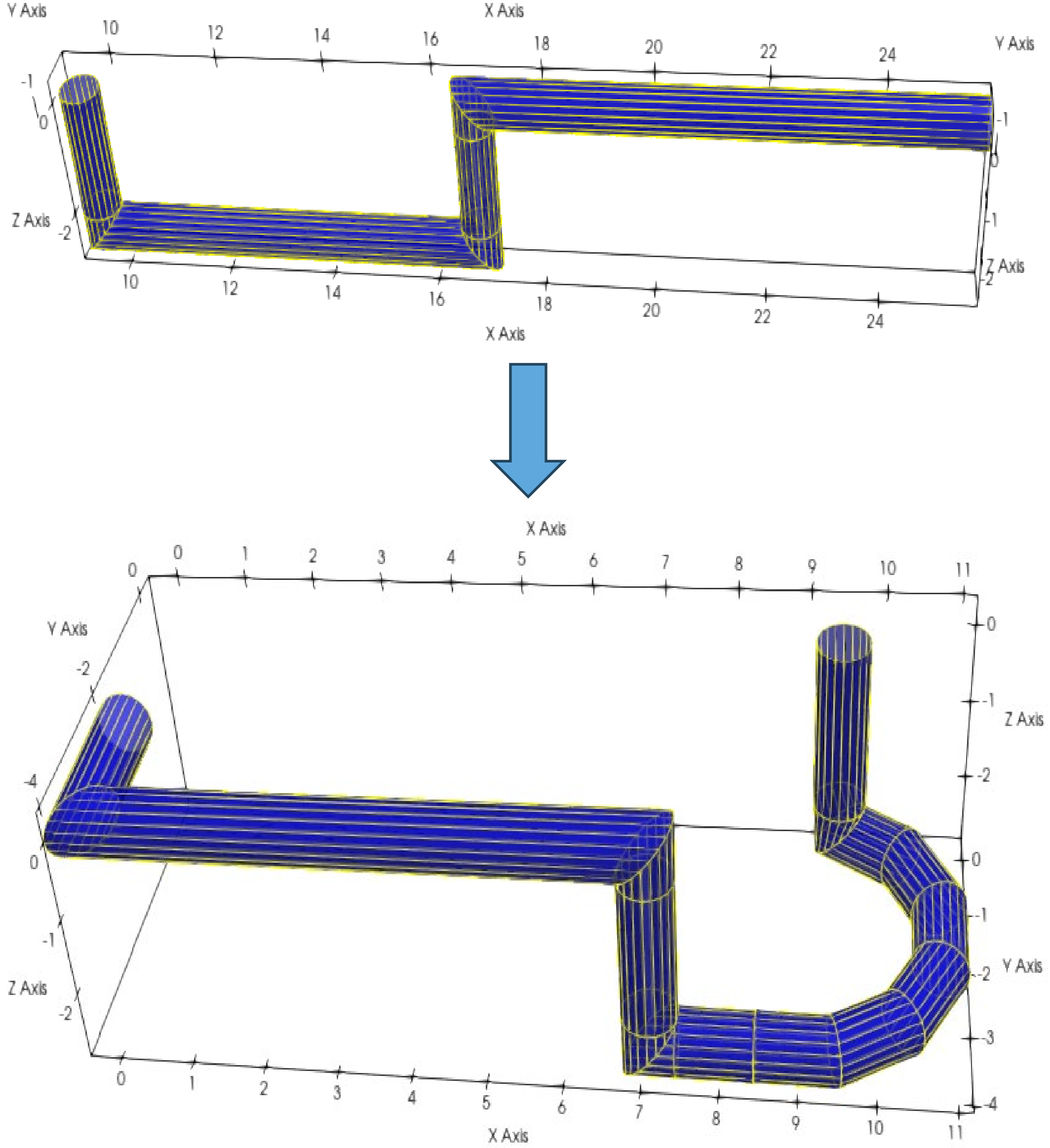
- **Motivation**: Extend ATHLET by 3D information
  - Compact 3D graphical system representation
  - Future usage of 3D data by physical models (e.g. thermal radiation in 3D core)
- **Basic geometry information** derived from CW TOPOLOGY
- Additional 3D data from **optional extension of PW GEOMETRY**
  - **rotation angle Φ in XY plane**
- Optional input under **new PW POSITION**
  - Rotation angle and (x,y,z) coordinate at TFO origin
  - Parameters to define if data are absolute or relative to preceeding TFO
  - Positioning of first TFO of each TFD system
  - Easy copying of TFOs with different spatial orientation
  - Note: changes in height position influence TH simulation

```
C---- OBJECT
 . . .
----- GEOMETRY
@  SG0   Z0   D0   A0   V0   DEP0   PHI
    :     :    :    :    :     :     :
 . . .
----- POSITION
@  PHI_P   IPHIFIX
   90.     0
@  X0    Y0    Z0   IPOSFIX
   1.    0.    0.   0
```

Example for Definition of 3D Data

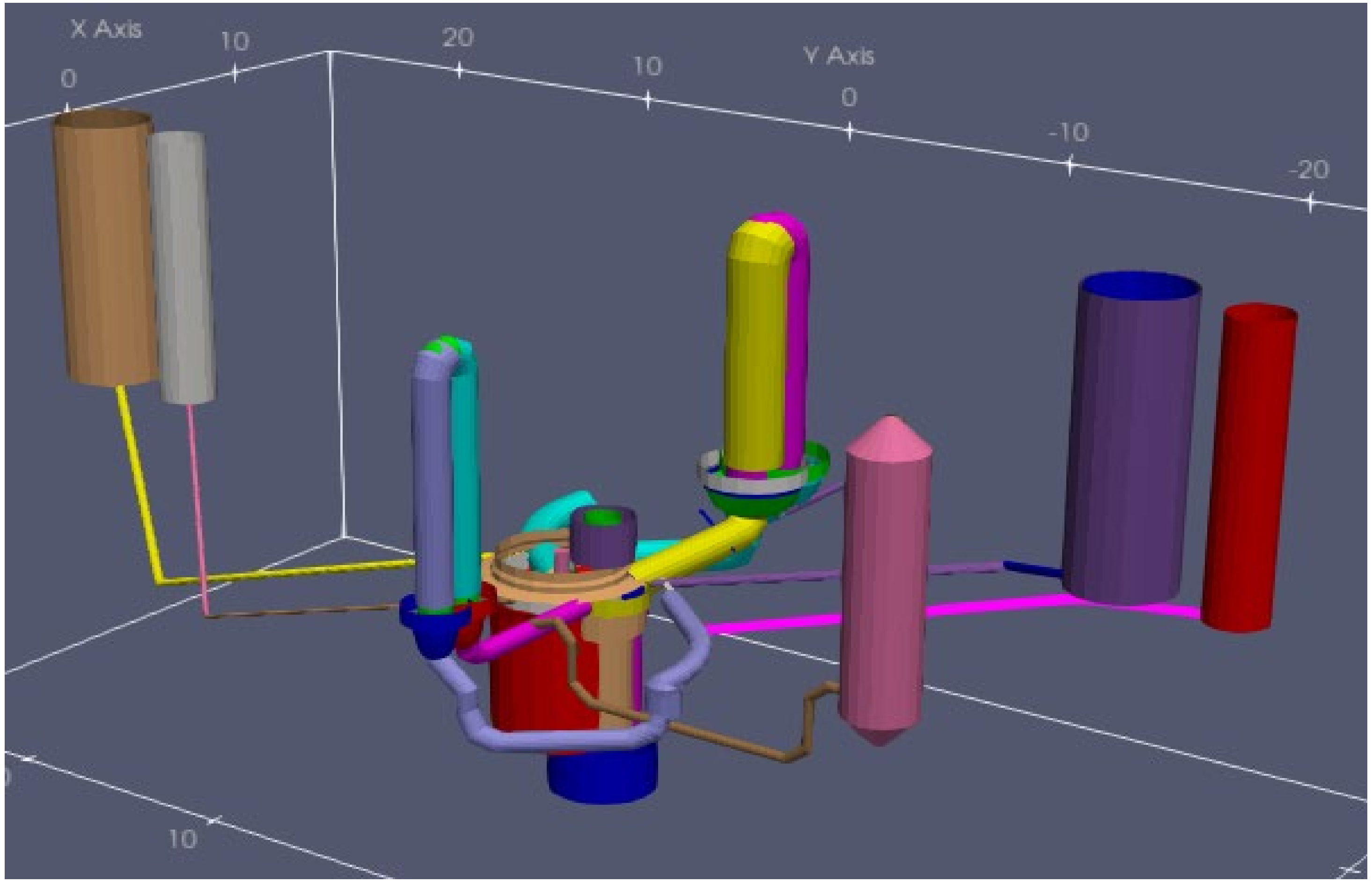
```
C---- PLUGIN
   vtk
. . .
C---- OBJECT
. . .
----- GEOMETRY
@      S0      Z0       D0     A0     V0    DEP0      PHI
    0.0      0.0     0.75    0.0    0.0    0.0      0.0
    2.5     -2.5     0.75    0.0    0.0    0.0    -30.0
    3.5     -2.5     0.75    0.0    0.0    0.0    -30.0
    4.5     -2.5     0.75    0.0    0.0    0.0    -30.0
    5.5     -2.5     0.75    0.0    0.0    0.0    -30.0
    6.5     -2.5     0.75    0.0    0.0    0.0    -30.0
    7.5     -2.5     0.75    0.0    0.0    0.0    -30.0
    8.5     -2.5     0.75    0.0    0.0    0.0      0.0
    9.5     -2.5     0.75    0.0    0.0    0.0      0.0
    9.84    -2.5     0.75    0.0    0.0    0.0      0.0
   12.34     0.0     0.75    0.0    0.0    0.0      0.0
   19.5      0.0     0.75    0.0    0.0    0.0    -90.0
   21.27     0.0     0.75    0.0    0.0    0.0      0.0
```

See sample1_VTK.in



VTK Plug-in

- Plug-in provided for generation of 3D object data in VTK format
- Enables visualization in ParaView
- All objects, TFOs and HCOs, represented by cylinders



PWR Sample

New Input Option: Improved Control of Friction Loss Adaption

During SSC, input values for friction and form loss coefficients can be adapted by ATHLET

- control by input parameters `IZETA0` and `IPRI0`
- to achieve a consistent state of the system
- Previously, a constant adaptation factor has been applied to all junctions within a priority chain

```
K---- PIPE
@  ITYPO        FPARO      ICMPO
   20           1.         0
. . .
----- FRICTION
. . .
----- SSCFRIC
@     FADAPT
      0.
@     SJO          FADAPTJ
      1.0          0.2
      3.5          1.
```

- Possibility to **restrict the adaptation to areas where information on pressure loss are incomplete** or unreliable
- **NEW PW SSCFRIC** under CW `OBJECT`
  - **FADAPT** switches on/off the adaptation for the complete TFO (PIPE or SJP)
  - `0.≤`**FADAPTJ**`≤1.` (de-)activates adaptation for individual junction near to position `SJ0` (with given weight)
  - Overwrites PC-wide settings by `IZETA0` and `IPRI0`

New Input Data Options and Checks

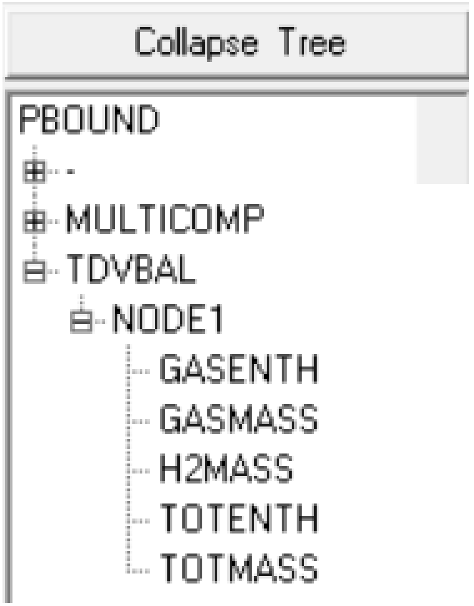
- **Optional SW under TOPOLOGY** to switch on/off sets of priority chains
  - Improved configuration control, also via PARAMETERS
- **New GCSM controller types** allow specification of real-valued constants (`CONST`) and logical constants (`LCONST`)
- Input check for **unused parameters**
  - **New optional PW `IDLE_PARAM`** under CW `SERVICES`
  - Quality assurance by detecting inadvertent input errors
- Additional input check for FUNGEN controller without X2NAME
  - IOPT must be -2 or 0
  - other options for IOPT cause a program stop now

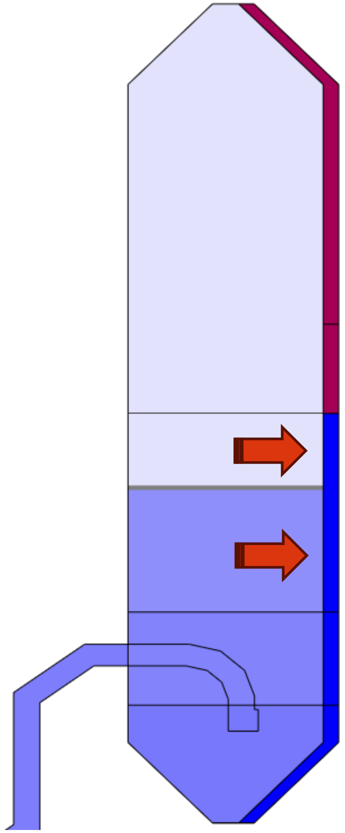
```
C---- PARAMETERS
CONFIG_1 = S*---
CONFIG_2 = S----
C---- TOPOLOGY
@     PRIORITY CHAINS
%CONFIG_1% COARSE
----- LOOP1
 . . .
%CONFIG_2% FINE
----- LOOP1A
 . . .
----- LOOP1B
 . . .
```

```
S---- SPRAY TEMPERATURE
@     YNAME     CONTYPE    X1NAME    X2NAME    X3NAME    X4NAME
      STSPRAY   FUNGEN     TIME      -         TTSPRAY   -
@     IOPT      GAIN       A1        A2        A3        A4
      0         1.         0.        0.        0.        0.
```

Additional Output Quantities

- **Integrated quantities for every TDV** (keyword `TDVBAL`)
  - Total (gas) mass and enthalpy flow towards/from the TDV
  - Mass flow per NC gas component
- Extended **balance quantities for TFD system** (`TFDGENERAL`)
  - Energy loss (`ENLOSS`): Integrated energy flow from TFD system into all connected HCOs except RODs and STEAMGENs
  - Total mass per NC gas component (e.g. `NITMASS`, `OXYGENMASS`,…)
- **HECU mixture level output under `ML_LEFT` or `ML_RIGHT`**
  - For mixture levels defined in TFOs on left/right side
  - Heat flows to sub-CVs QHLUP and QHLOW provided separately
  - Additional output for HTC, MODE, etc. for sub-CV above ML

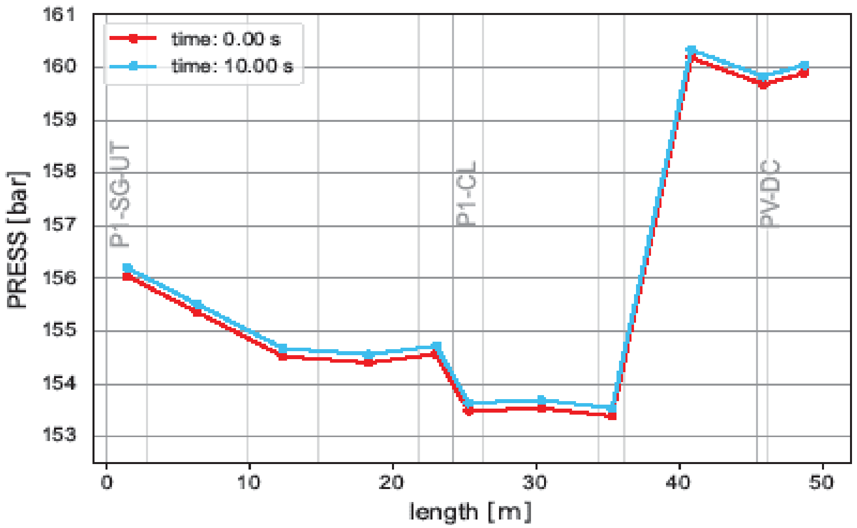


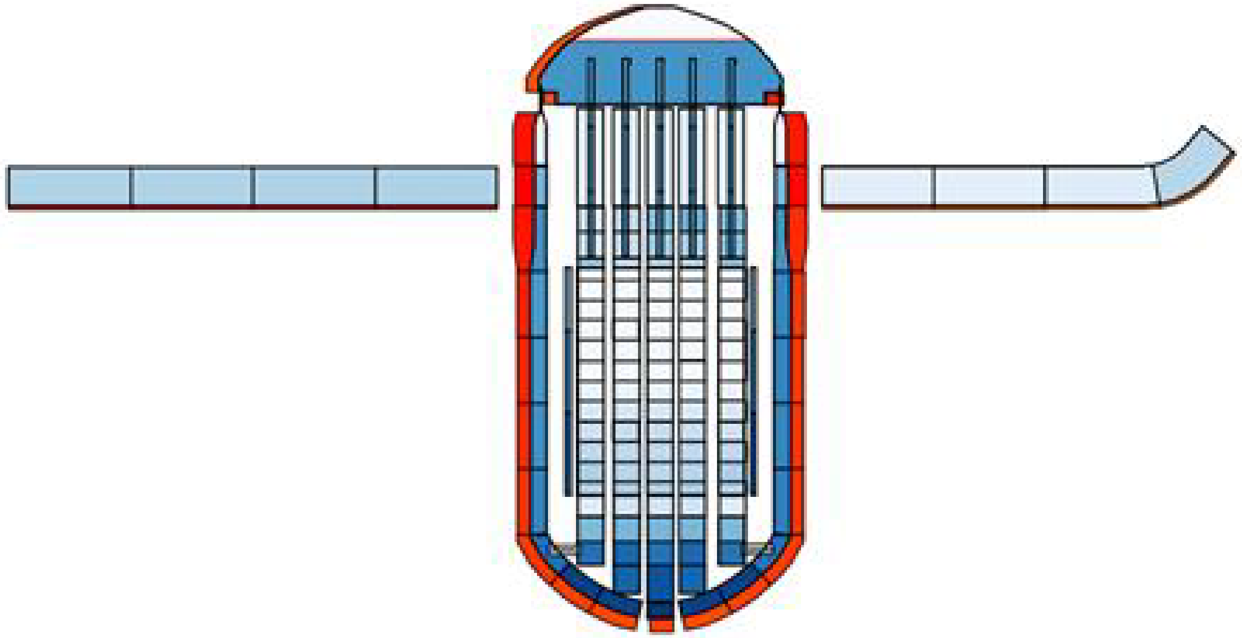


ML_LEFT	I/J	IMLHL	INDHL	QHLUP	QHLLOW	QLUP	QLLOW	HTCL	HTCVL	HTCCOL	HTCMIL	MODEL
	1	9	1	2.89E+06	7.18E+05	2.89E+06	7.18E+05	0.00E+00	0.00E+00	0.00E+00	4.39E+04	25

Batchplot Plotting Tool

- Python based plotting tool for hdf5 and pd data
- **Platform independent**, for Linux and MS Windows
- Plotting **temporal, axial and radial (HCO) distributions**
- **New module to visualize 2D graphics from AIG**
  - Dynamic visualization via Jupyter notebook possible
  - For details and examples see Batchplot manual





Summary

- **Numerous new and improved models in ATHLET 3.5**
  - Various new options for **detailed simulation of structures**, e.g. spacer grid model, 3D heat conduction, and new geometry type for horizonal plate
  - **New heat pipe module**, e.g. for investigation of **Micro Modular Reactors**
  - Improved modelling for **flow regimes and friction losses**
  - **User support and quality assurance** by extended input checks and output data
  - On-going integration of ATHLET and ATHLET-CD

➡ See **ATHLET Program Updates Manual** for complete listing

Thank you for your attention!

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Gesellschaft für Anlagen- und
Reaktorsicherheit (GRS) gGmbH
Schwertnergasse 1
50667 Köln

www.grs.de

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