

Developments of HCP

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Second Joint ICTP-IAEA Workshop on Open-Source Nuclear Codes for Reactor Analysis
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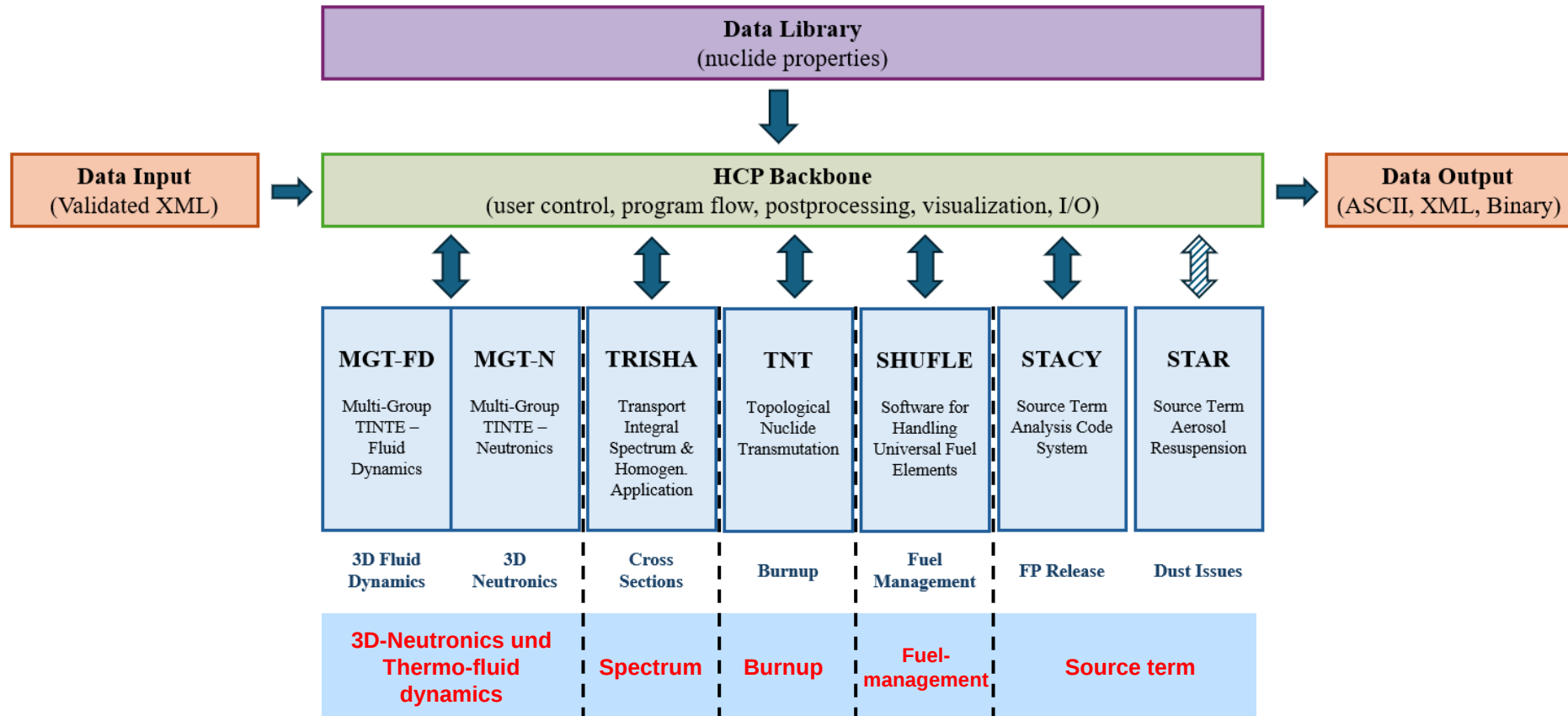
Overview

- Introduction of the HTR Code Package (HCP)
- Progress in the research project KONHCP I
 - Implementation of control rod
 - IT work
- Outlook for the research project KONHCP II
 - Implementation of molten salt coolant
 - Implementation of prismatic geometry
 - Further integration of the STACY module
- Advances in Independent Research
 - Conductive heat transfer calculation
 - LibGen fixing and I/O improvement
 - Benchmark and safety analysis
- HCP Demonstration, Application, and User Forum
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A unique integrated code system for the numerical simulation of the core of the high-temperature reactor (HTR)



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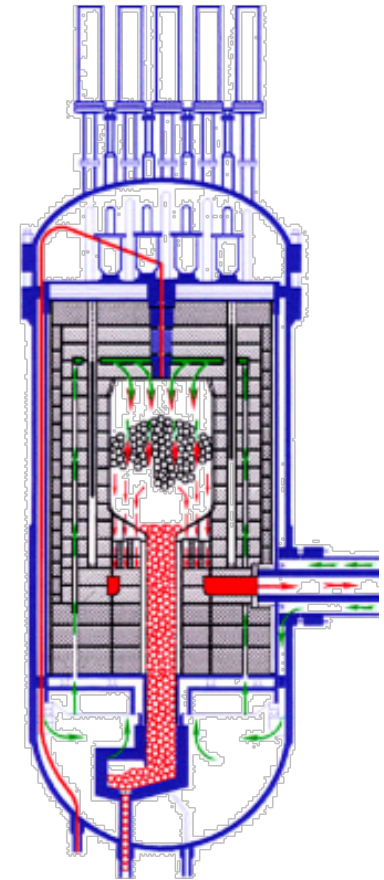
Reactor	<u>PR500</u>	<u>HTR10</u>	PBMR	MHTR250
TP (MW)	500	10	400	2*250
ASS	S1	S2	S2	S2
Reactor	<u>AVR</u>	<u>THTR</u>	HTR-100	<u>HTR-PM</u>
TP (MW)	50	750	100	2*250
ASS	Rods in noses	S1	S2	S2

TP: Thermal power

ASS: Shut down system

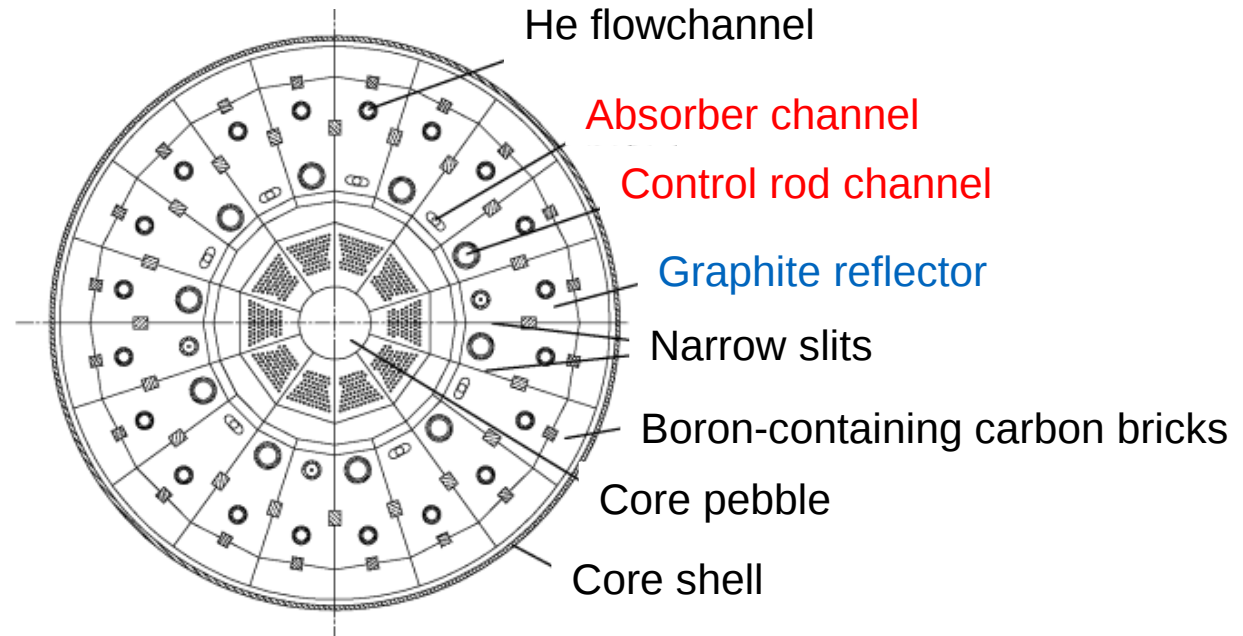
S1: Reflector rods + core rods

S2: Reflector rods + reflector small absorber pebbles



HTR-10

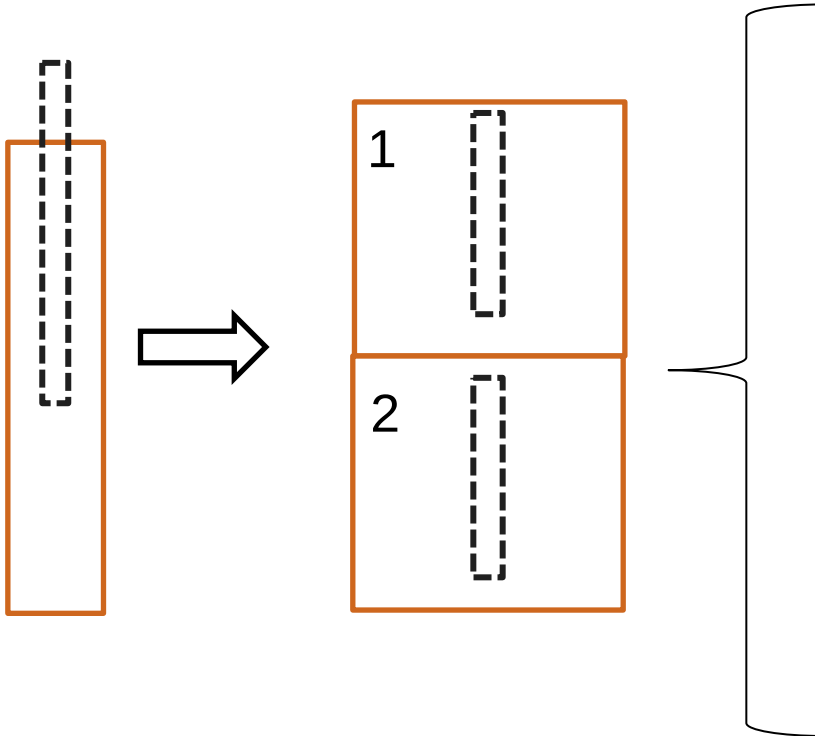
The cross-section of the reactor core



Rod insert logic:

Introducing reactivity by changing the nuclide amount or add new nuclides in the node

Control rod movement simulation



Model.xml

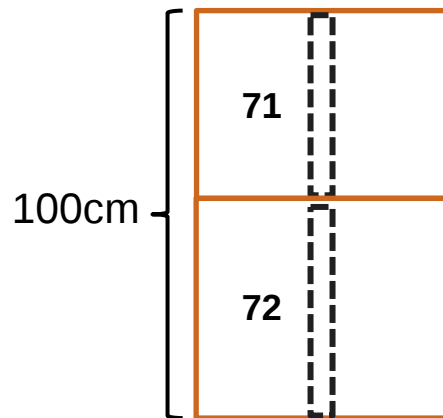
Definition of a component type, mainly to enable

1. the user to define the **position** of the control rod channel in the core
2. the user to define the insertion **depth**
3. Define the **shape, material composition** of the rod

Scenario.xml

Define rod **insertion depth** and time for **transient** as an action

Method 1



```
<Action begin="1.0" end="1.0" unit="s">
  <Calculation type="Stationary" mode="manual">
    <Ramp type="NuclideConcentration">
      <NuclideConcentration node="71">
        <Amount nuclide="B-10" unit="1/barn/cm"> 9.64977E-04 </Amount>
      </NuclideConcentration>
    </Ramp>
    <Ramp type="NuclideConcentration">
      <NuclideConcentration node="72">
        <Amount nuclide="B-10" unit="1/barn/cm"> 9.64977E-04 </Amount>
      </NuclideConcentration>
    </Ramp>
```

Method 2

```
<Ramp duration="100.0" unit="s" type="Nuclear">
  <Nuclear type="ControlRod">
    <ControlRod shape="0" value="100.0" unit="cm"/>
  </Nuclear>
</Ramp>
```

Identify nodes automatically

Each mesh in the control rod region is composed of three batches: two solid batches: the unmovable reflector (batch_1) and the control rod hole to be inserted (batch_2), and one fluid batch (batch_3) representing the remaining cavity space.

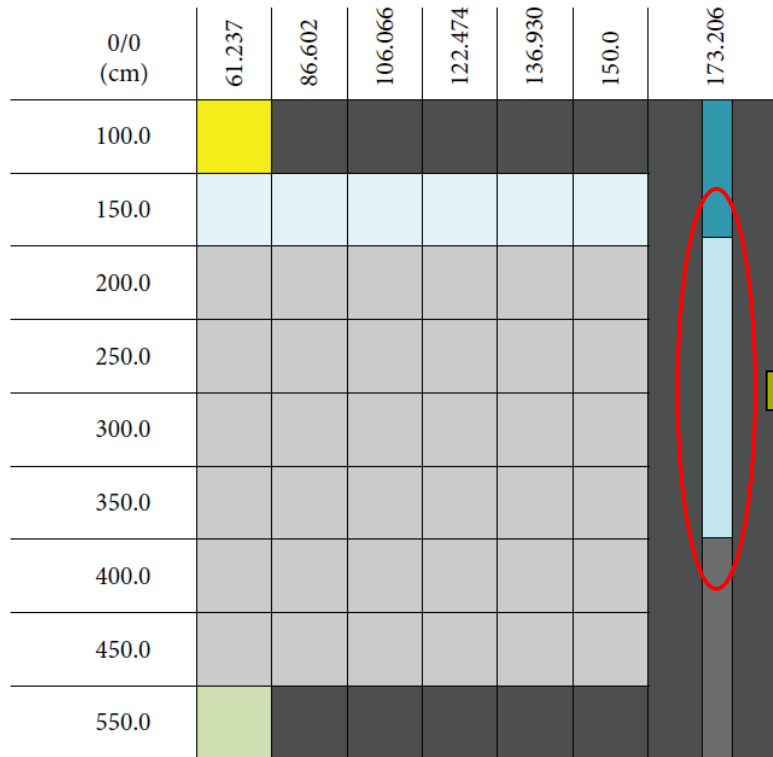
Batch volume test in HCP:

$$V_t \geq V_{\text{rod}}$$

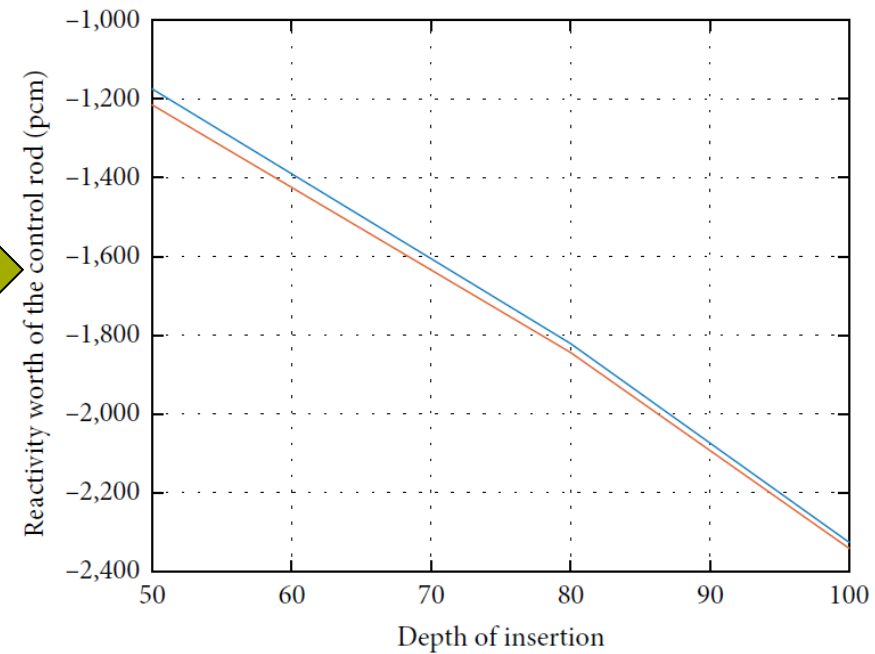
$$V_t \geq V_{\text{batch_2}}$$

$$V_t - V_{\text{batch_1}} \geq V_{\text{batch_2}} \geq V_{\text{rod}}$$

Verification



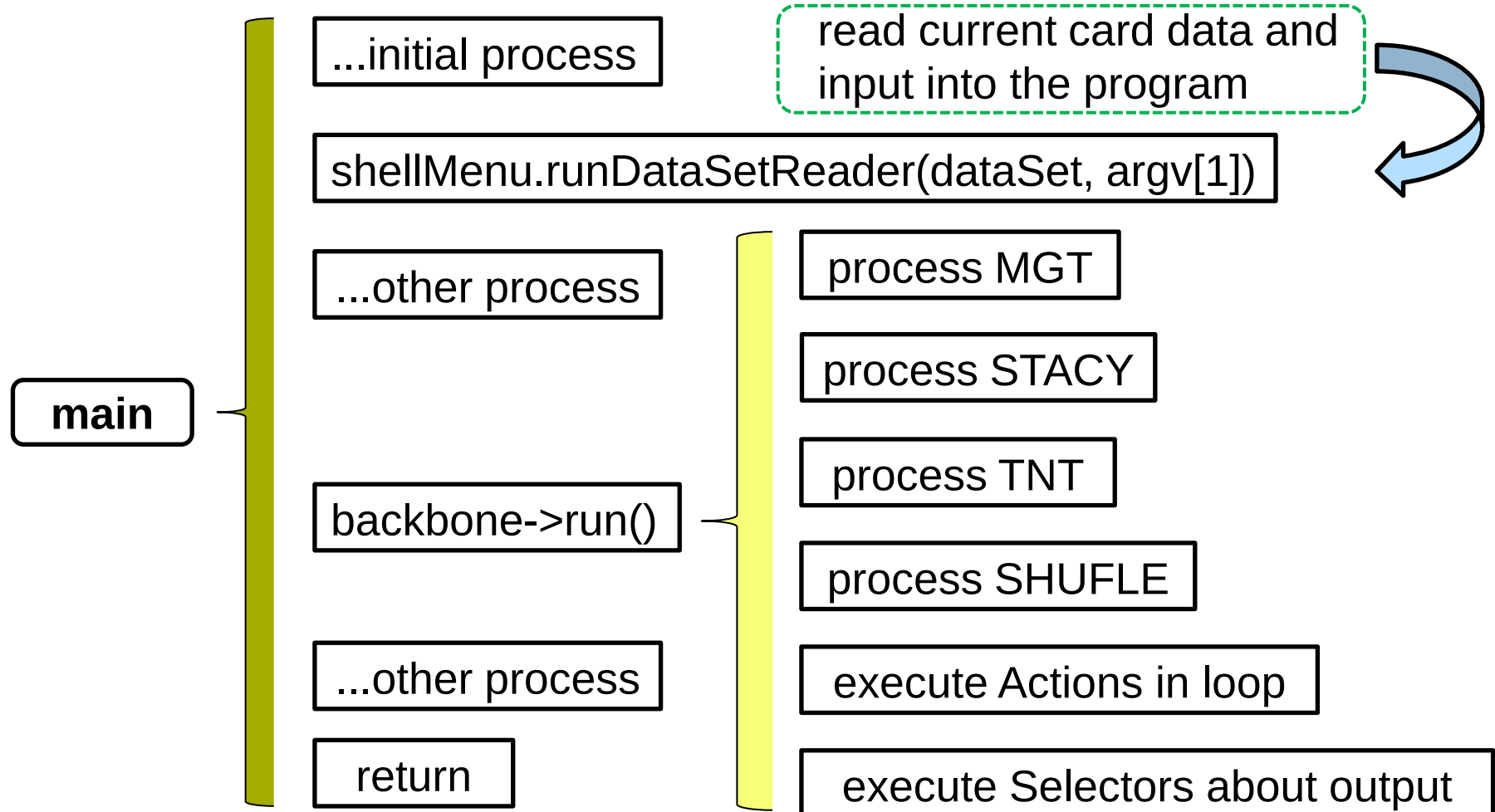
- Rod drive
- Rod cavity
- Pebble bed
- Sink
- Source
- Cavity flow
- Reflector

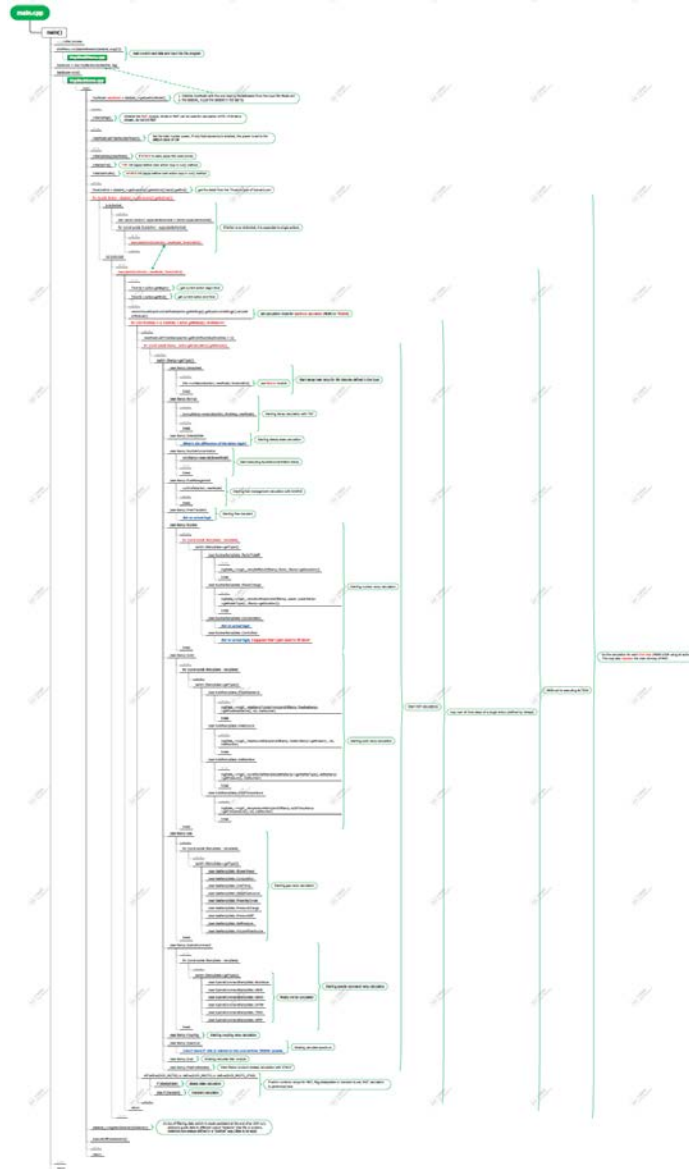


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The main code structure of HCP





- Construction of project **hosting warehouse** based on **Gitlab**

Administrator > HCP2 > Repository

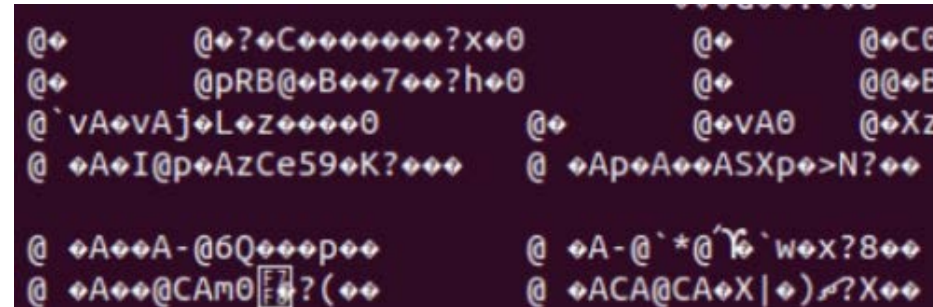
master hcp2 / code / + ▾

History Find file Web IDE ⬇ ▾ Clone ▾

 **hcp2 of IAEA**
root authored 6 days ago 252e3b59 🔒

Name	Last commit	Last update
..		
bin	hcp2 of IAEA	6 days ago
data	hcp2 of IAEA	6 days ago
libs	hcp2 of IAEA	6 days ago
src	hcp2 of IAEA	6 days ago
tests	hcp2 of IAEA	6 days ago
tools	hcp2 of IAEA	6 days ago
vendor	hcp2 of IAEA	6 days ago
CMakeLists.txt	hcp2 of IAEA	6 days ago
old_CMakeLists.txt	hcp2 of IAEA	6 days ago

- Locate some **memory leak** points as shown below



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NaF-ZrF₄ selected: high heat transfer capability

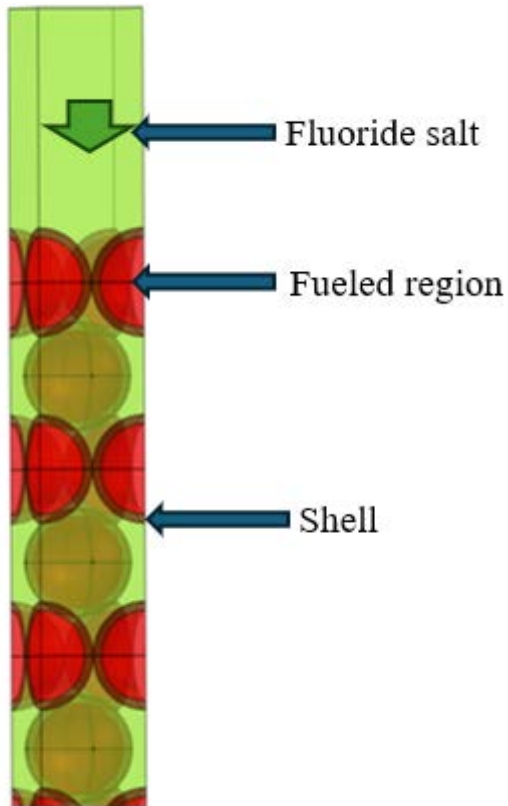
Comparison of thermal and neutron characteristics of different fluoride salts.

Coolant	Composition (molar ratio)	Heat transfer characteristics (700 °C)					Neutron characteristics	
		Specific heat capacity $C_p/J \cdot$ $kg^{-1} \cdot K^{-1}$	Melting point/°C	Density $\rho/$ $kg \cdot m^{-3}$	Turbulent forced convection FOM ^a	Turbulent natural convection FOM ^a	Total neutron capture (per unit volume) relative to graphite	Moderating ratio (avg. Over 0.1–10eV)
Na (550 °C)	–	1267.8	97.72	820	13.15	20	47	2
H ₂ O(300 °C)	–	5732.1	0	720	0.20	4.8	75	246
LiF–BeF ₂	67:33	2414.2	460	1940	0.70	13.9	8	60
NaF–BeF ₂	57:43	2175.7	340	2010	0.91	16.5	28	15
NaF–ZrF ₄	59.5:40.5	1171.5	500	3140	1.98	14.7	24	10
LiF–NaF–ZrF ₄	22:55:23	1255.2	436	2790	1.42	13.9	20	13
LiF–NaF–KF	46.5:11.5:42	1884.1	454	2020	1.13	13.3	90	2

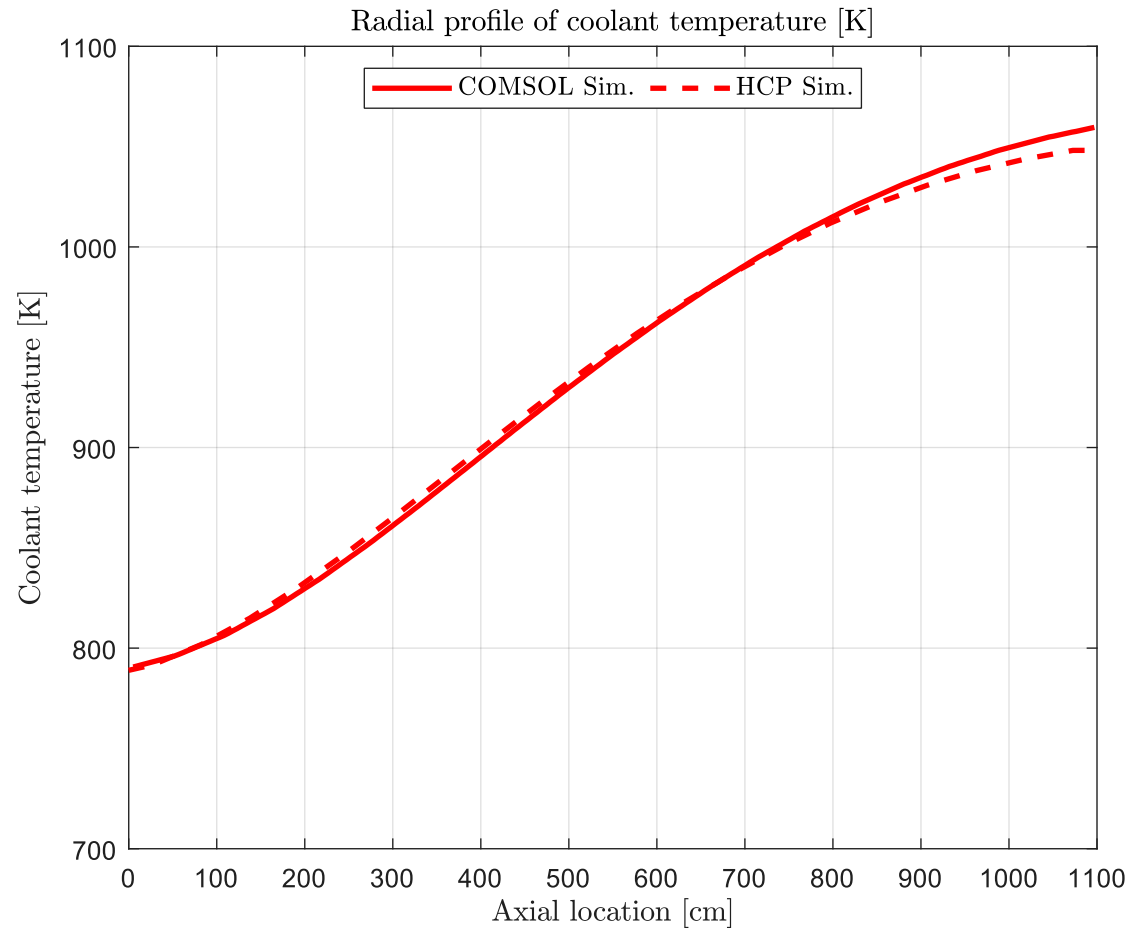
Note a: FOM is a comprehensive constant for judging the heat transfer performance of turbulent and natural convection. The larger the value, the stronger the heat transfer capacity.

Jiang, D., Zhang, D., Li, X., Wang, S., Wang, C., Qin, H., ... & Qiu, S. (2022). Fluoride-salt-cooled high-temperature reactors: Review of historical milestones, research status, challenges, and outlook. Renewable and Sustainable Energy Reviews, 161, 112345.

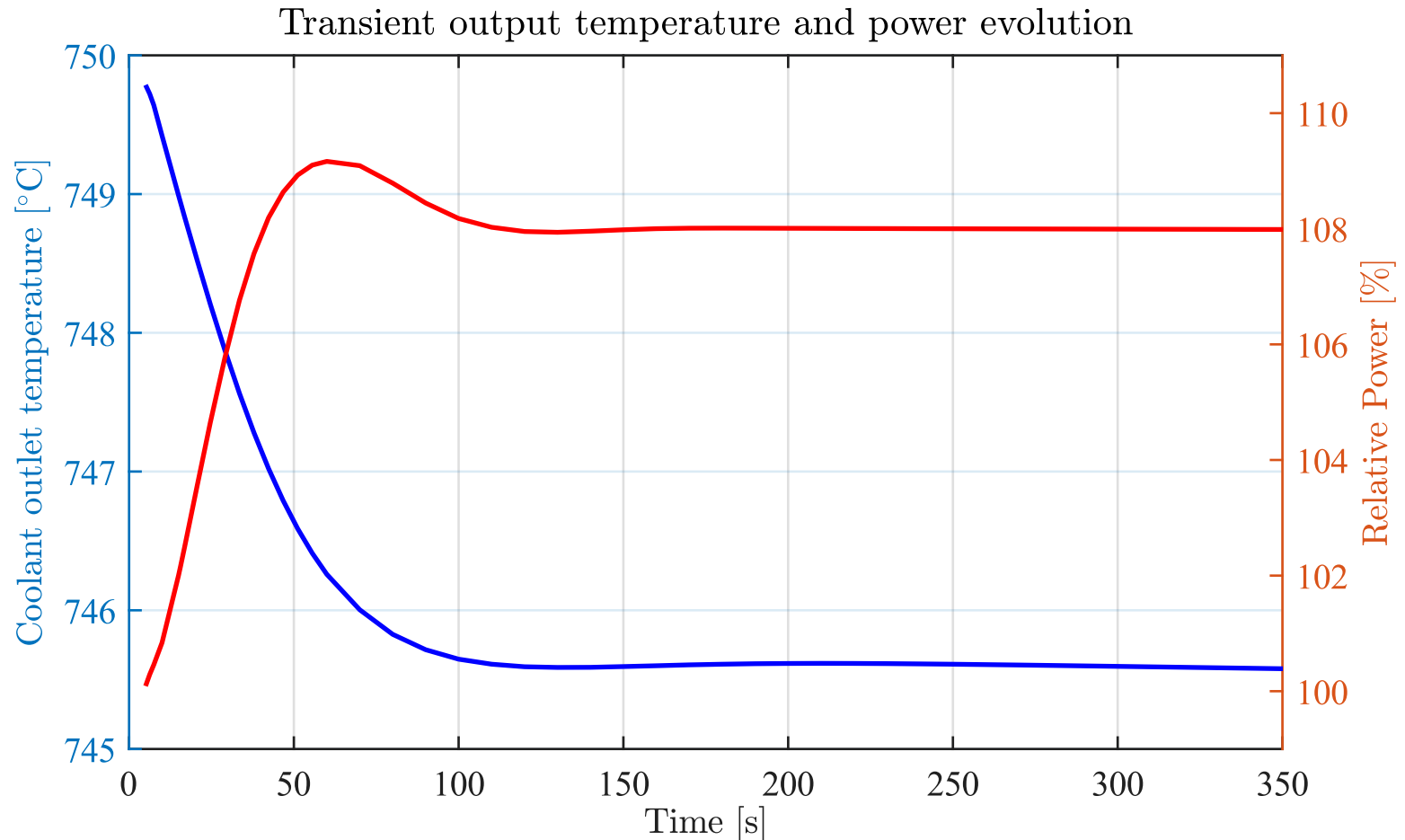
Benchmark: coolant temperature distribution in hot channel (SS)



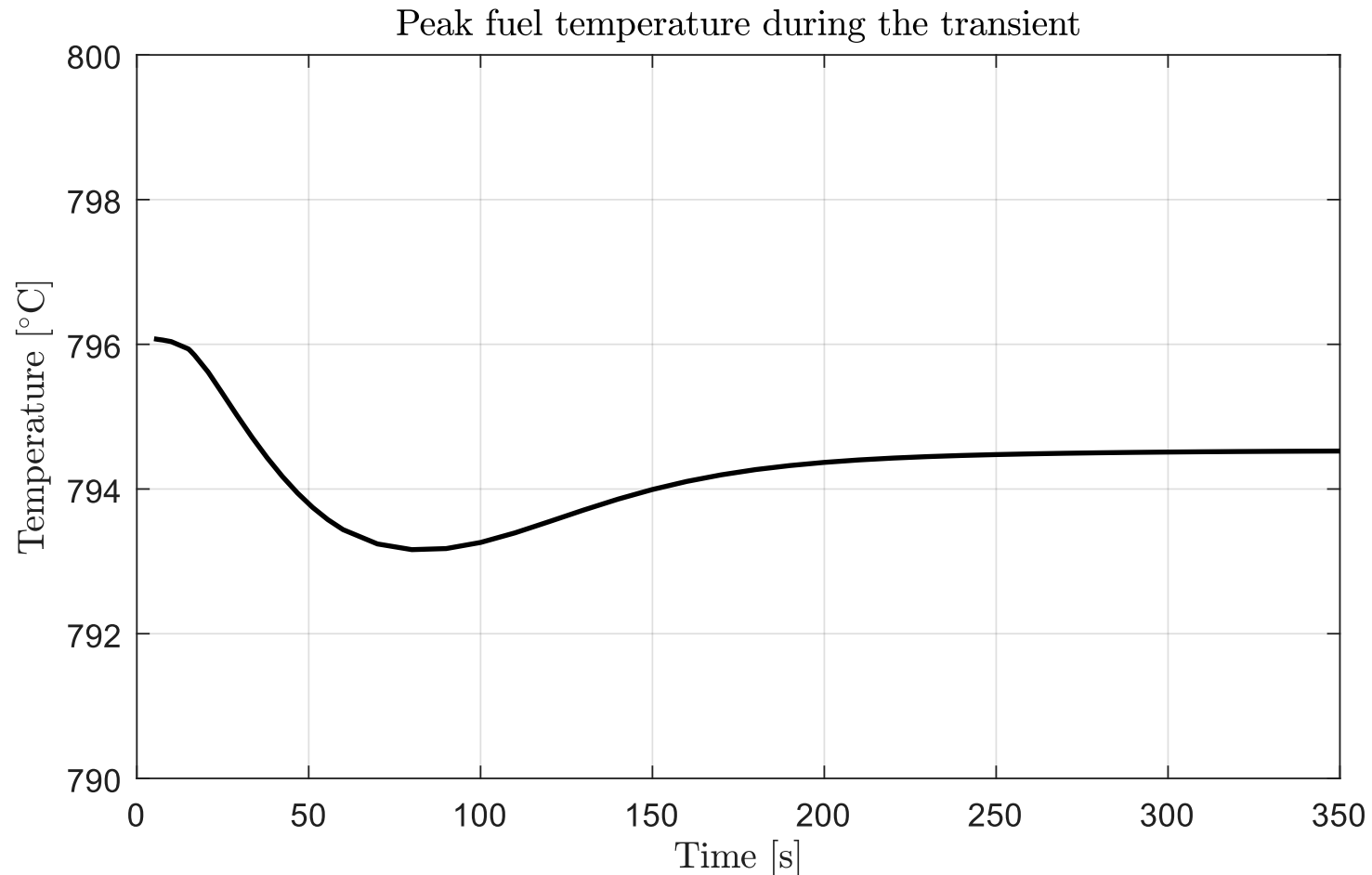
COMSOL model



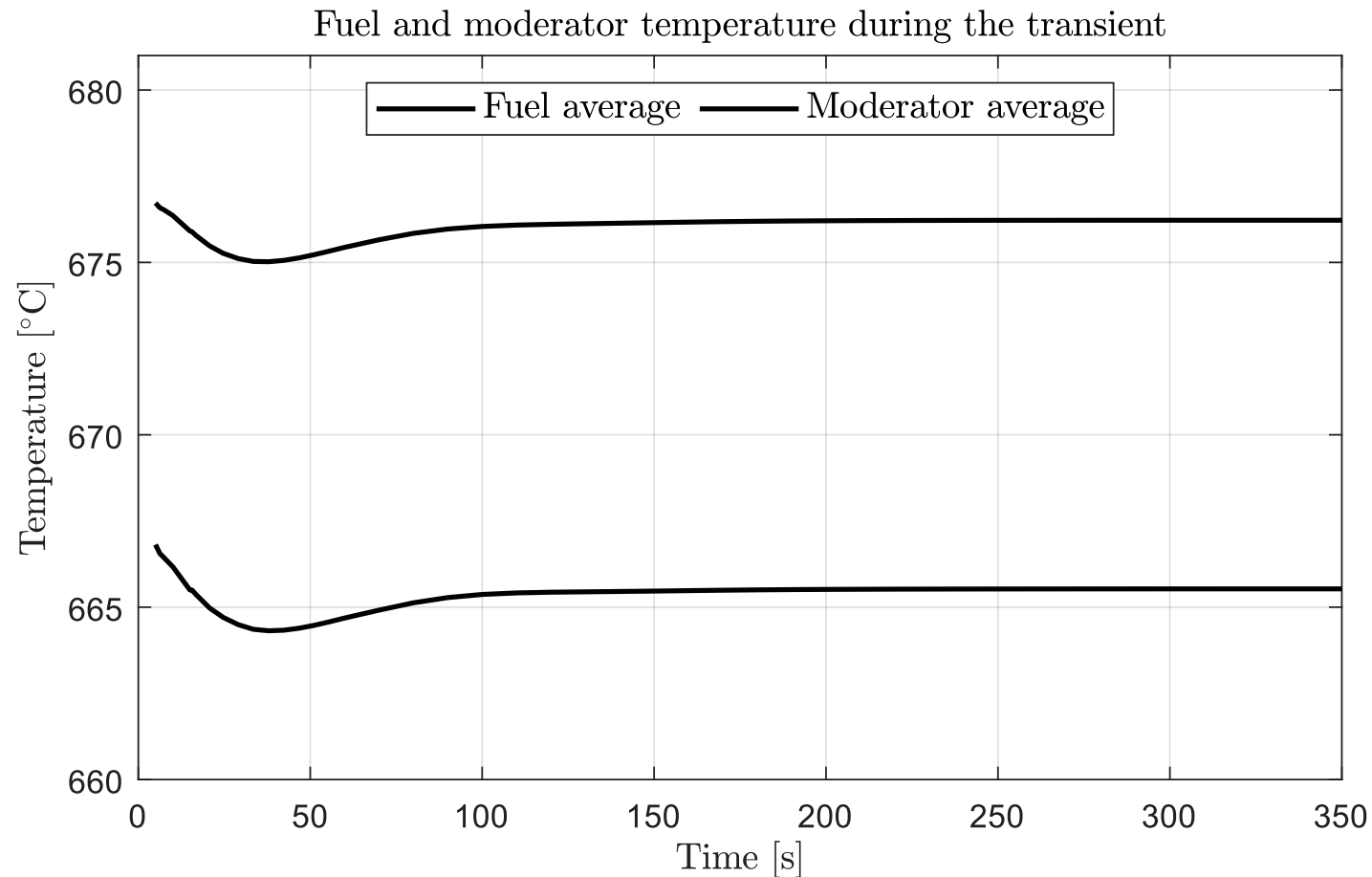
Transient of coolant mass flow rate variation:
+10% in 10 seconds



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1. Considerations for geometry

- Input reading: “prisBlock” already defined in ModelReader.cpp, but nuclide vectors cannot be assigned (only spherical supported for now), extension needed
- Class definition: extend the existing classes to include the prismatic block structure and hexagonal mesh (datamodel -> fuel element related files)
- Material properties: already defined in “SpecificHeat.f90”
- Transfer hexagonal meshes from backbone to MGT directly, high accuracy, but solver has to be adjusted
- Trick: implement a subroutine in backbone to map prismatic blocks between hexagonal meshes and cylindrical meshes, MGT will only see cylindrical meshes and do calculation as usual

2. Considerations for neutronics calculation

- Governing equations unchanged
- Multiple fuel/coolant channels in one block: homogenization
- Spatial discretization of control volumes has to be adjusted for hexagonal mesh: FDM -> FEM?
- Special attention for irregular outer boundary

3. Considerations for thermal-hydraulics calculation

- Governing equations unchanged
- Convective heat transfer in coolant channels, conductive heat transfer between blocks
- Dedicated constitutive models have to be added
- Same issue for discretization

4. Considerations for burnup calculation

- Take batch-wise nuclide inventory and flux distribution directly from backbone
- No modification expected

5. Considerations for control rod

- SHUFLE module for control rod movement, movable solid volume inside the prismatic block (as fuel element)
- Maybe a little modification for the fuel element volume division and a correction factor for coolant channels

6. Considerations for nuclear data library

- Different correction methods for geometric heterogeneities
- Some influences on the accuracy, but not urgent

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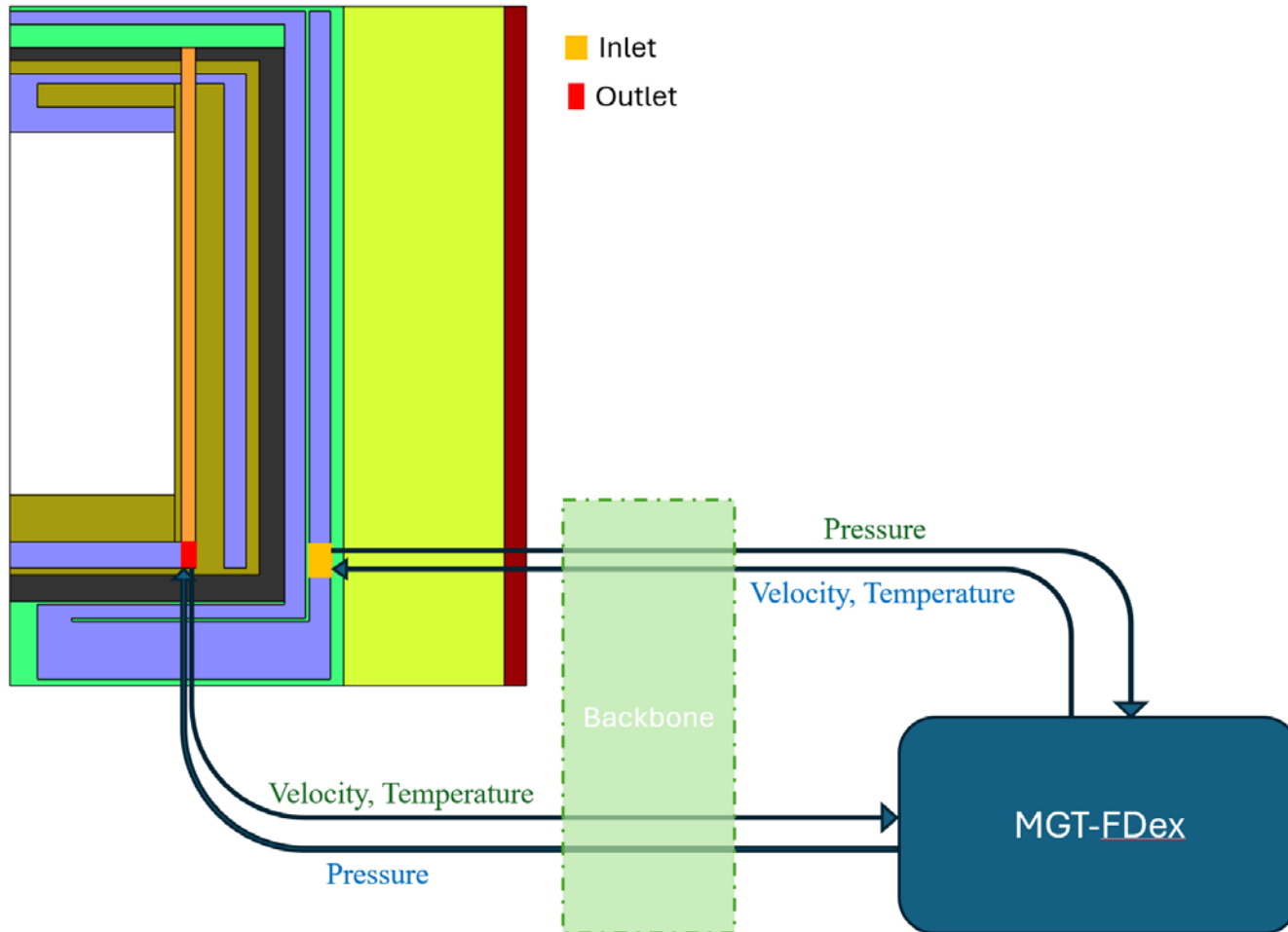
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This part will be conducted at **Becker Technologies**.

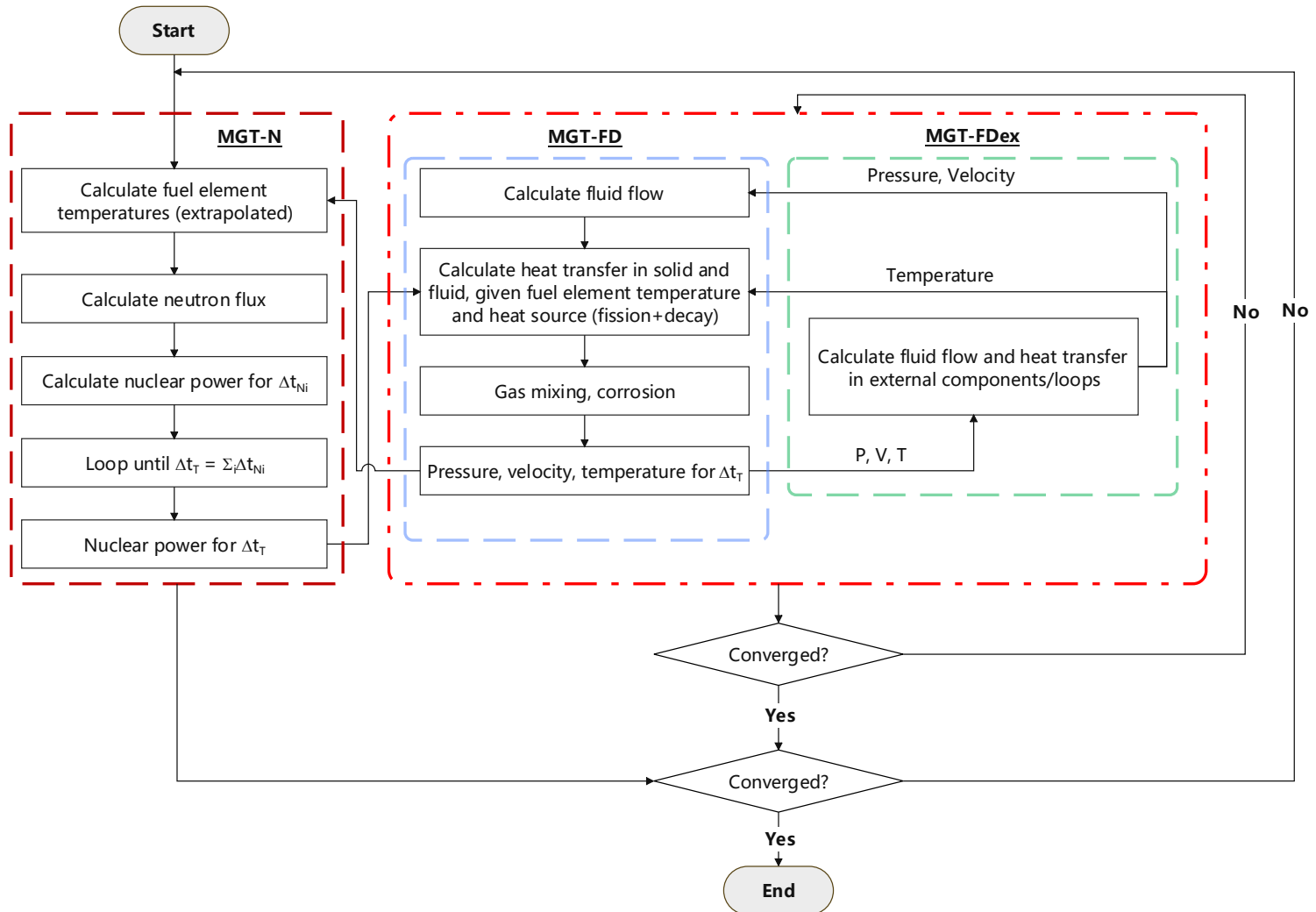
- Continuation of the integration of the source term calculation module STACY
- Extension of the STACY module to the prismatic core
- Integration of the STAR module

- Plan A:
 - Integrate the external components into the calculation chain of MGT-FD
 - Apply the lumped parameter method to perform 0D (point-wise) calculation of each component, implicit coupled with the core
 - Straightforward and convergent
 - Low accuracy and resolution, limited capacity
- Plan B:
 - Develop a new module: MGT-FDex
 - 1D calculation, explicit coupling: exchange of boundary parameters through backbone (mesh overlapping)
 - More properties of “component” needed: nodalization, junction, flow chain, thermal coupling...
 - No change of MGT-FD, modular feature
 - High accuracy and resolution, more flexible

Schematic of mesh overlapping:



Code structure for coupling:

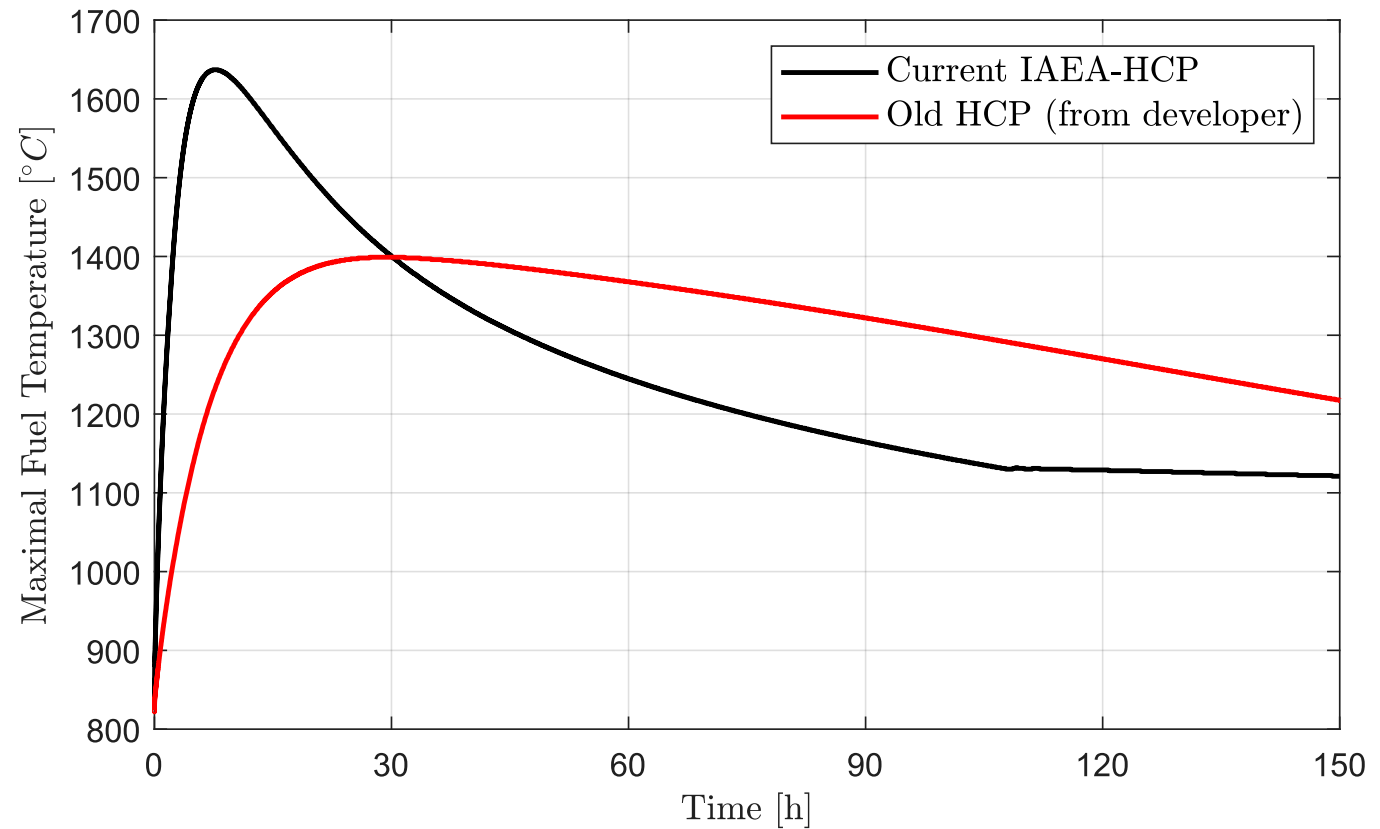


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DLOFC transient: HTR-MODUL-200

Same input deck!

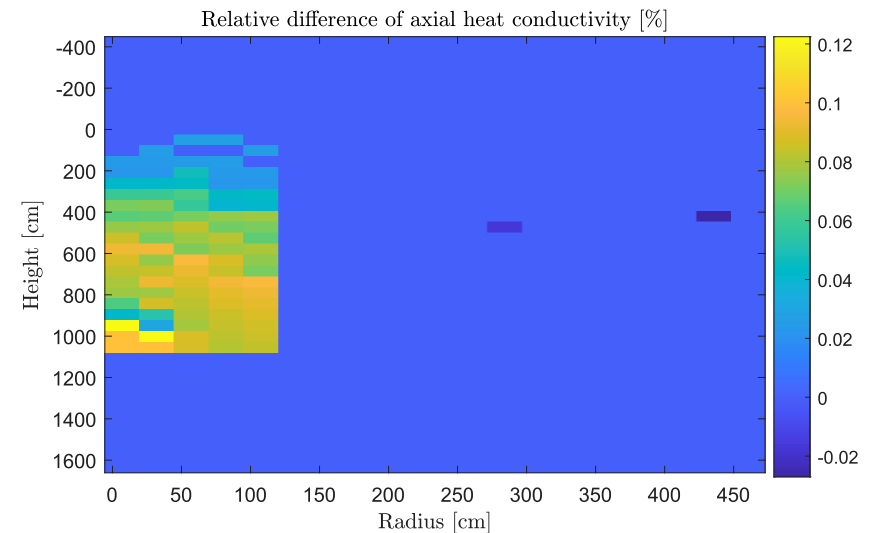
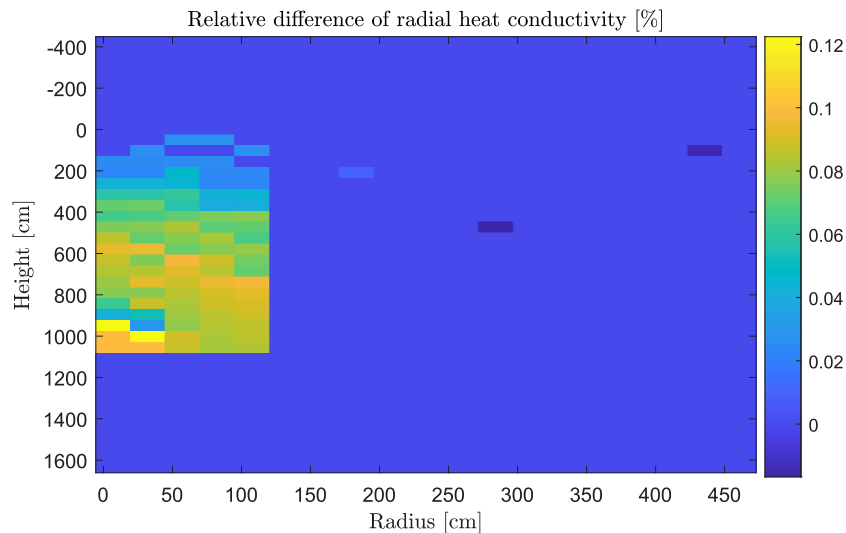


DLOFC transient: HTR-MODUL-200, output comparison

1. Same or similar at $t=0$: Moderator temperature, fuel temperature, gas pressure, gas flow, gas conduction, gas boundary temperature, Reynolds number, heat transfer coefficient, solid temperature, fuel element temperature, power distribution
2. Different at $t=0$: **Radial heat conductivity, Axial heat conductivity**

DLOFC transient: HTR-MODUL-200, output comparison

Radial heat conductivity and Axial heat conductivity



In the active zone (core), the heat conductivity is underestimated by around 10% -> 8°C difference

DLOFC transient: Meshing

Heat conductivity mapping



Heat conductivity law distribution of meshes:

phi layer: 0

z / r	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
0	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	G03	G03	M02
1	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	G03	G03	M02
2	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	G03	G03	M02
3	R13	R13	R13	R13	R13	R13	R13	R03	R13	R13	R13	R13	R13	R13	M02	M02	M02	G03	G03	M02
4	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
5	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
6	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
7	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
8	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
9	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
10	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
11	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
12	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
13	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
14	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
15	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
16	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
17	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
18	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
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20	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
21	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
22	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
23	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
24	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
25	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
26	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
27	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
28	L03A	L03A	L03A	L03A	L03A	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
29	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	G03	G03	M02
30	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	VAL	G03	M02
31	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	VAL	G03	M02
32	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	VAL	G03	M02
33	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	VAL	G03	M02
34	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	M02	M02	M02	VAL	G03	M02
35	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	G03	M02
36	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	G03	M02
37	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	G03	M02
38	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	G03	M02
39	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	G03	M02

Legend:

G03 : Nitrogen (ref: JUEL-1362, Dec. 1976)
L03A : Maximum of Zehner/Schlunder and Robold, pebble material A3-3 matrix graphite, irradiated
M02 : V2A steel, DIN 4541 (ref: Thyssen)
R03 : Reactor graphite, Grade A (ref: company SGL)
R13 : Carbon brick, according to Lukasewicz
VAL : Fixed input value

DLOFC transient: Meshing

Heat capacity mapping



```
<Component id="1" type="PebbleBed" label="Pebble bed">
  <Property type="SolidTemperature" unit="C"> 510.0 </Property>
  <Property type="GasTemperature" unit="C"> 490.0 </Property>
  <Property type="FuelTempCalculation"> 1 </Property> <!-- Default value is false (Material
  <Property type="GraphiteForCorrosion" kind="rule" factor="1.0"> R03 </Property> <!-- acco
  <Property type="HeatConductivity" kind="rule" unit="W/cmK" factor="1.0"> L03A </Property>
  <Property type="Dose" unit="1021edn"> 1.5 </Property>
  <Property type="FuelElement"> 1 </Property> <!-- For a stand alone MGT run, use radiu:
  <Property type="GraphiteInGasContact"> 0.61 </Property>
  <Property type="FillingFactor" unit="normal"> 0.61 </Property>
</Component>
```

Heat capacity law distribution of meshes:

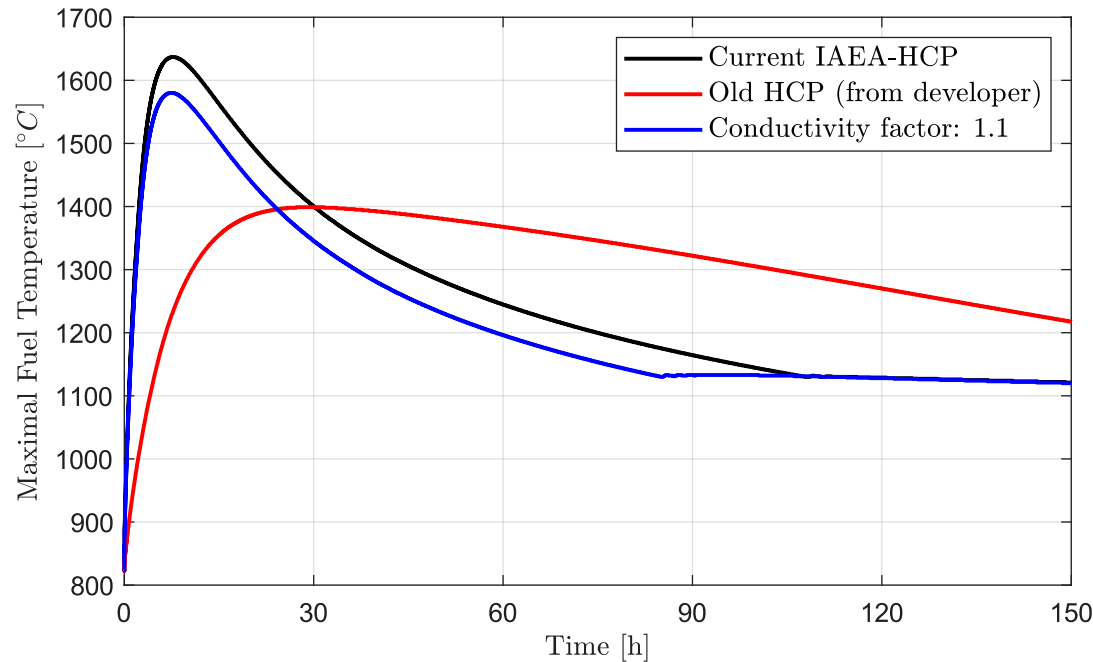
phi layer: 0

z / r	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
0	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL	VAL
1	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL
2	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL
3	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	M02	M02	M02	VAL	VAL
4	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
5	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
6	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
7	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
8	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
9	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
10	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
11	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
12	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
13	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
14	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
15	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
16	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
17	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
18	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
19	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
20	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
21	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
22	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
23	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
24	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
25	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
26	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
27	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
28	VAL	VAL	VAL	VAL	VAL	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
29	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
30	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
31	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
32	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
33	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R03	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
34	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	R13	M02	M02	M02	M02	VAL	VAL
35	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL
36	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL
37	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL
38	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL
39	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	M02	VAL	VAL

Legend:

M02 : V2A steel, DIN 4541 (ref: Thyssen)
 R03 : Reactor graphite SGL Grade A, NBG 10 (ref: FBMR)
 R13 : Carbon brick
 VAL : Fixed input value

DLOFC transient: HTR-MODUL-200, output comparison



Increase the heat conductivity in the active zone (core) by a factor of 1.1, lower peak, but worse timing.

DLOFC transient: HTR-MODUL-200, analysis

- Heat conductivity value has an influence, but not towards the right direction
- Test: Increase the formulas in *SpecificHeat.f90* by a factor of 100, but no change in results, specific heat not implemented!
- Check the results:
 - Old: 10s to 60s, 822 °C to 831°C, 9 °C/s
 - New: 10s to 60s, 830 °C to 863 °C, 33 °C/s
 - Specific heat value of R03 (graphite) material: 2.3 to 2.7 $J/cm^3 K$
 - Specific heat to be divided missing somewhere during the temperature calculation?

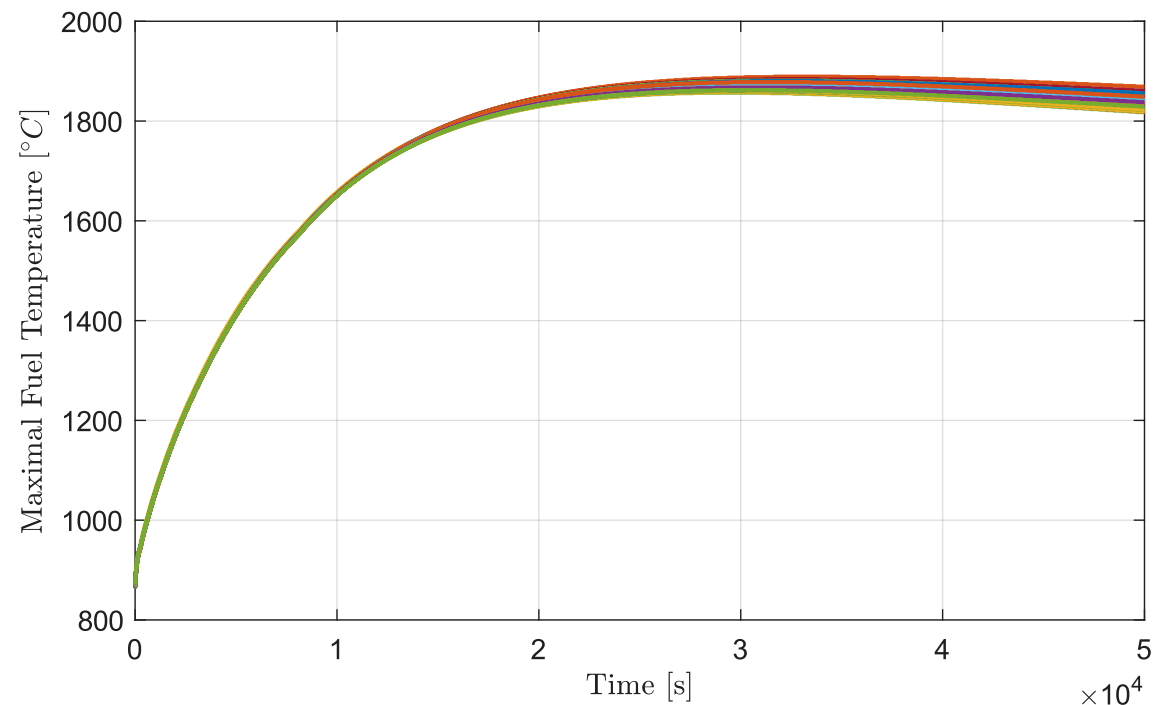
Uncertainty quantification of R03: conductivity & capacity

1. Sampling: two factor $\sim U(0.8, 1.2)$
2. Modification of the source code: *HeatConductivity.f90*, *SpecificHeat.f90*
3. Compile executable files: proto0001, proto0002, ... , proto0093
4. Perform simulations with same or different input decks with these executable files
5. Data extraction and post-processing, uncertainty/sensitivity analysis

Uncertainty quantification of R03: conductivity & capacity

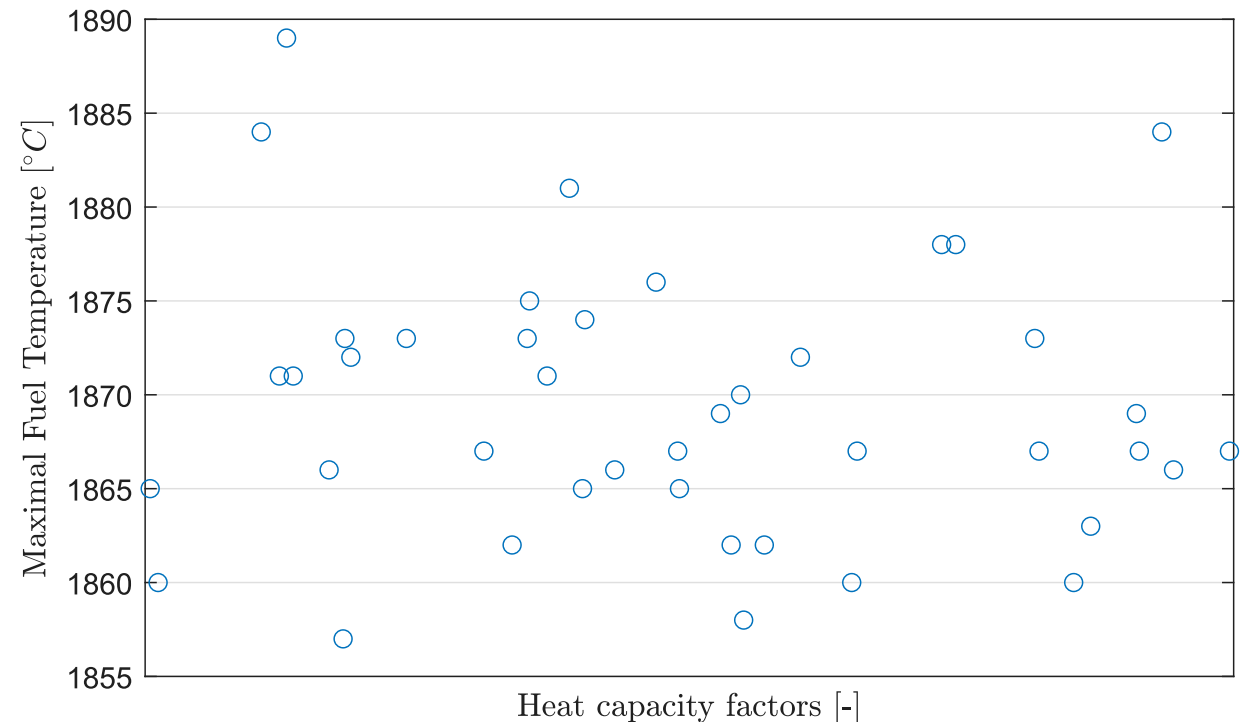
Factor of R03 heat conductivity $\sim U(0.8, 1.2)$

Factor of R03 heat capacity $\sim U(0.8, 1.2)$

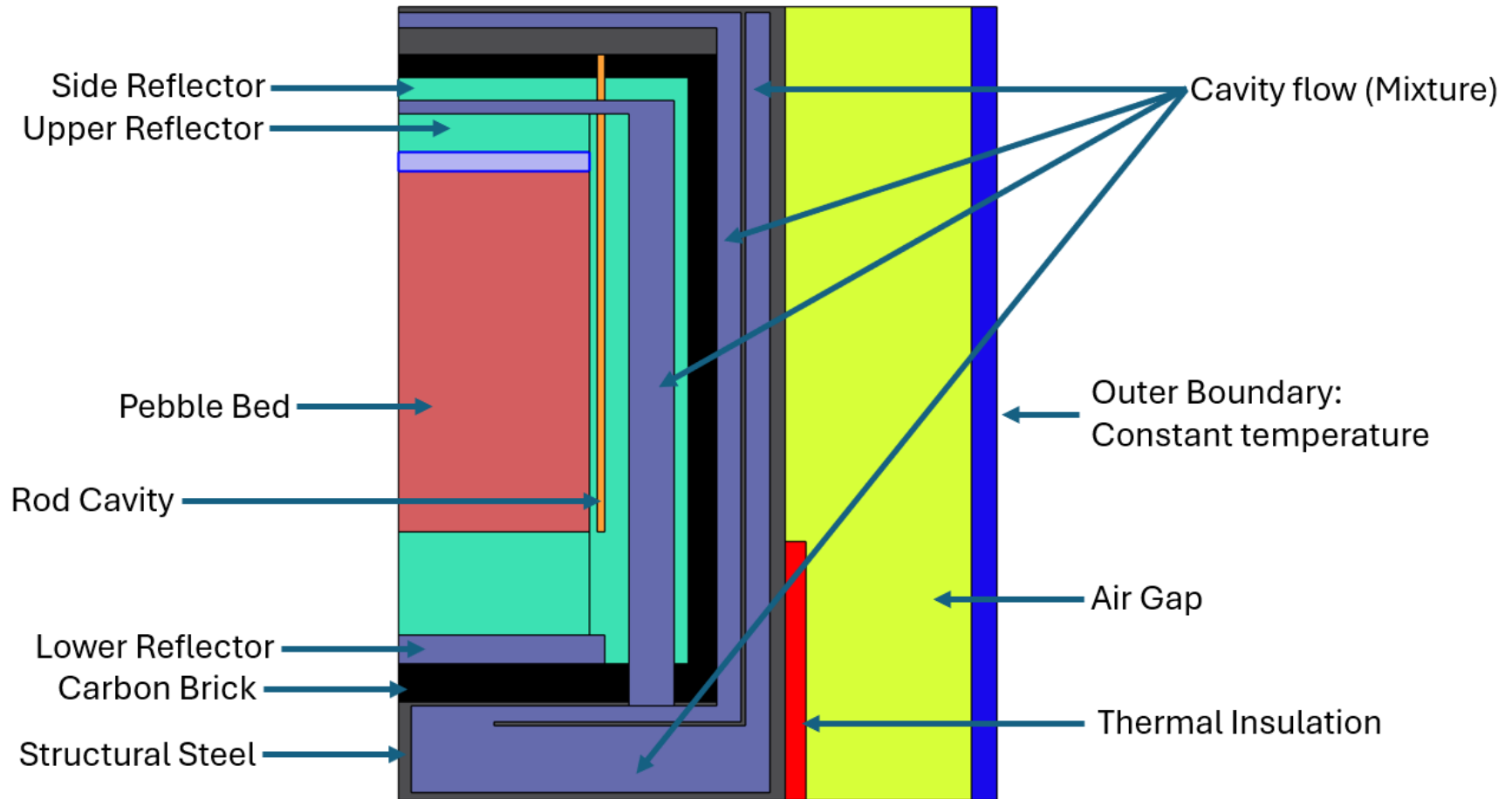


Uncertainty quantification of R03: conductivity & capacity

Factor of R03
heat capacity
-> not correlated!

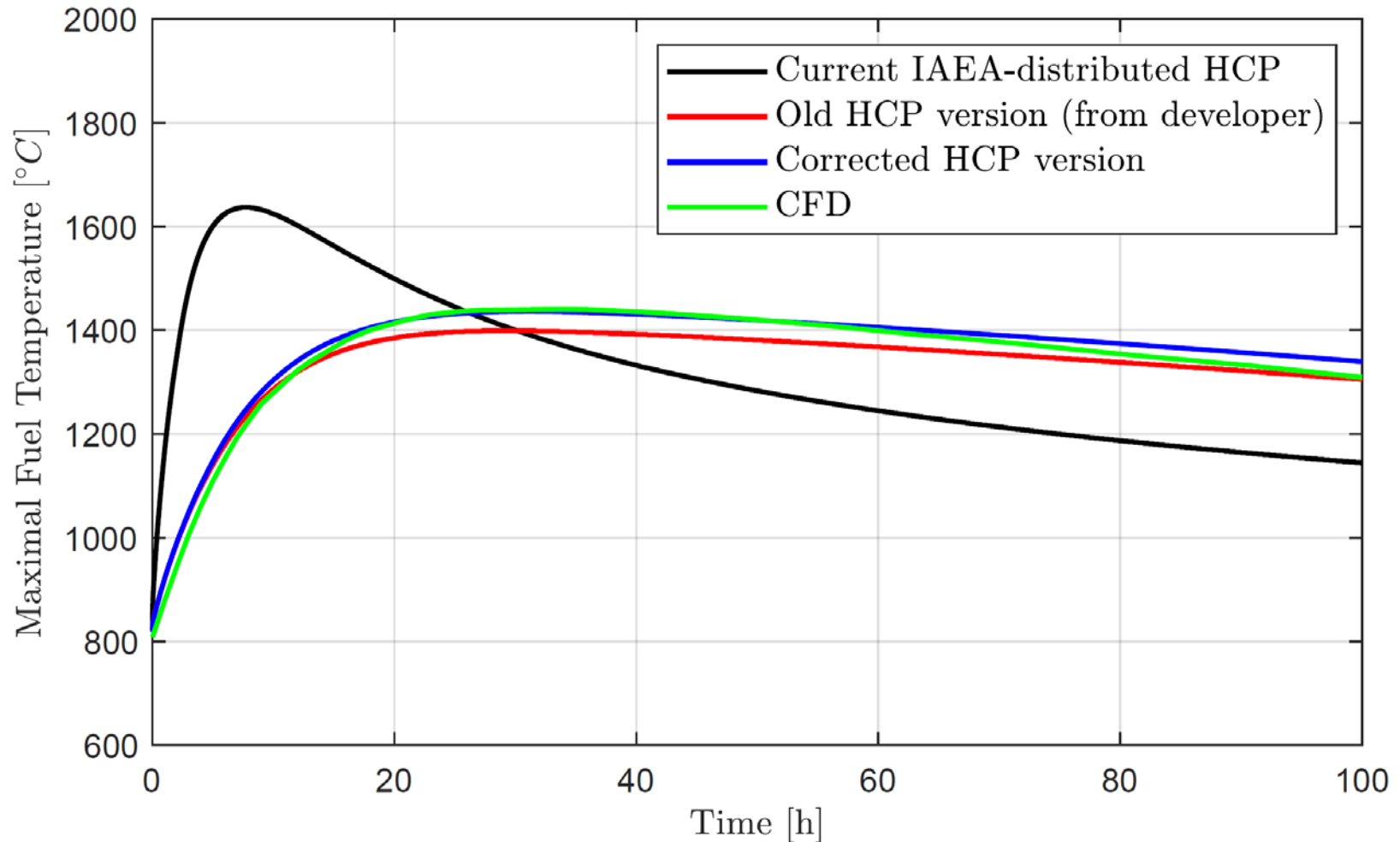


DLOFC transient: HTR-MODUL-200



COMSOL model

DLOFC transient: HTR-MODUL-200



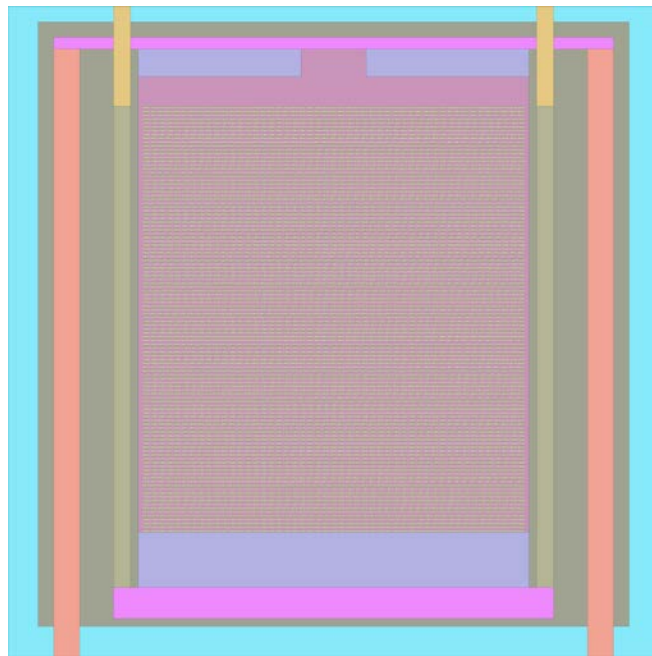
Overview

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No input folders: reverse-engineered

Error in subroutine “readFissionSpectrumData”: rewritten

Several libraries generated and benchmarked



Serpent model

HTR-PM keff values calculated using different nuclear data libraries

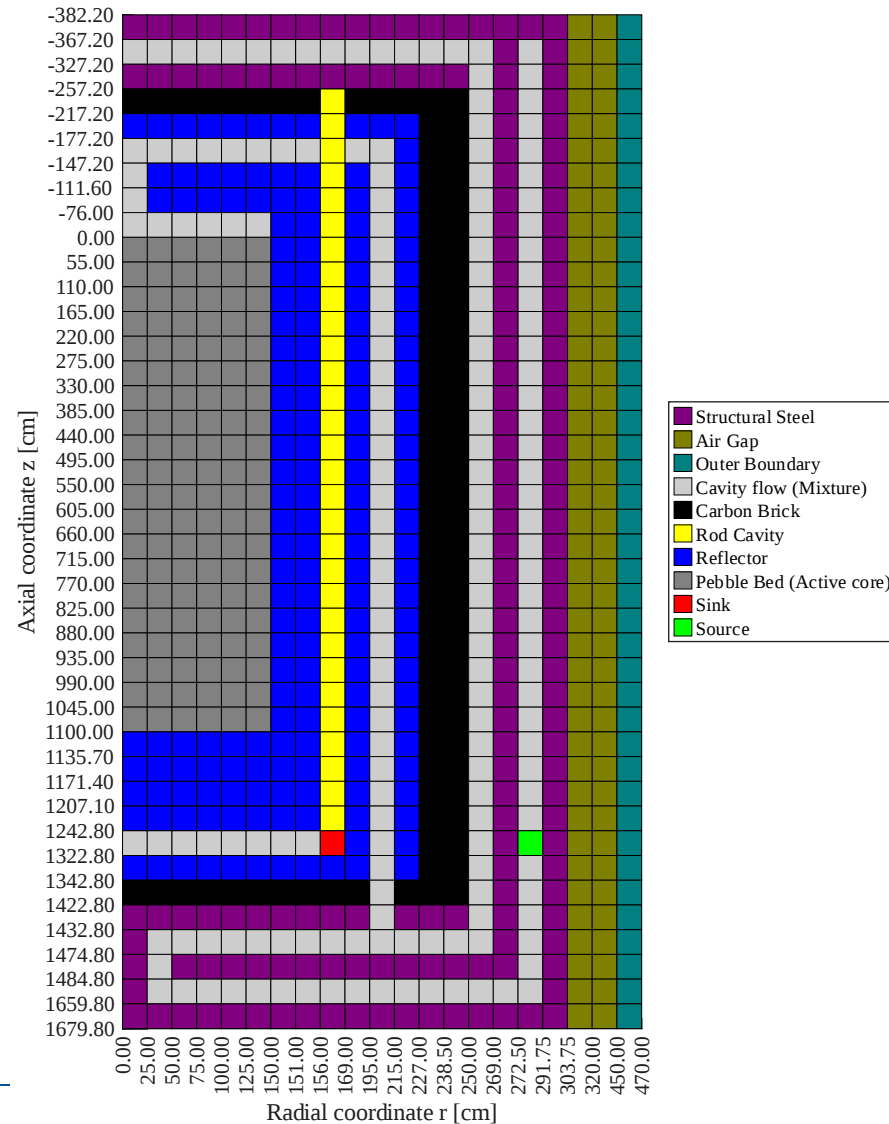
Coolant	Library	HCP	Serpent	Relative error [%]
Helium	ENDF/B-VII.0 (coarse)	1.34254	1.33417	0.627
	ENDF/B-VII.0 (fine)	1.34198	1.33417	0.585
	ENDF/B-VII.1 (fine)	1.33220	1.32555	0.502
	ENDF/B-VIII.0 (fine)	1.33792	1.32618	0.885
Air	ENDF/B-VII.0 (coarse)	1.34191	1.33041	0.864
	ENDF/B-VII.0 (fine)	1.34134	1.33041	0.822
	ENDF/B-VII.1 (fine)	1.33157	1.32236	0.694
	ENDF/B-VIII.0 (fine)	1.33730	1.32263	1.109

- Selector -> “Restart”, but power history missing -> **flaw in decay heat calculation!** -> external preprocessing code: add power history items automatically
- “Restart.xml” very large -> **not all the nuclides are crucial** for reactor dynamics (maybe important for STACY) -> external preprocessing code: filter to remove low density nuclides -> 126MB to 3MB without losing accuracy, faster
- **No output** for burnup calculation -> several functions in subroutine “TntOutputWriter” rewritten -> output: time-dependent batch-wise nuclide inventory
- Very limited transient data in “output.txt” -> binary file “data.ptr” -> data extraction through reverse-engineering -> but **only 1D** data -> extended to include time-dependent 3D data

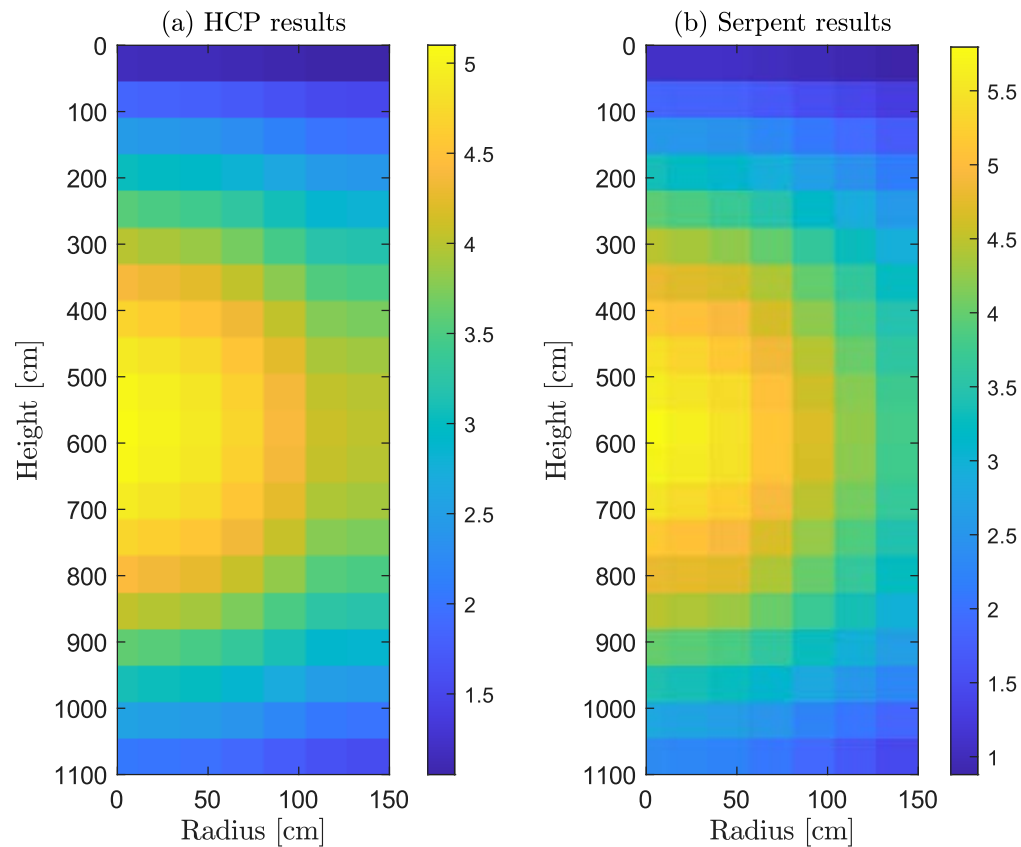
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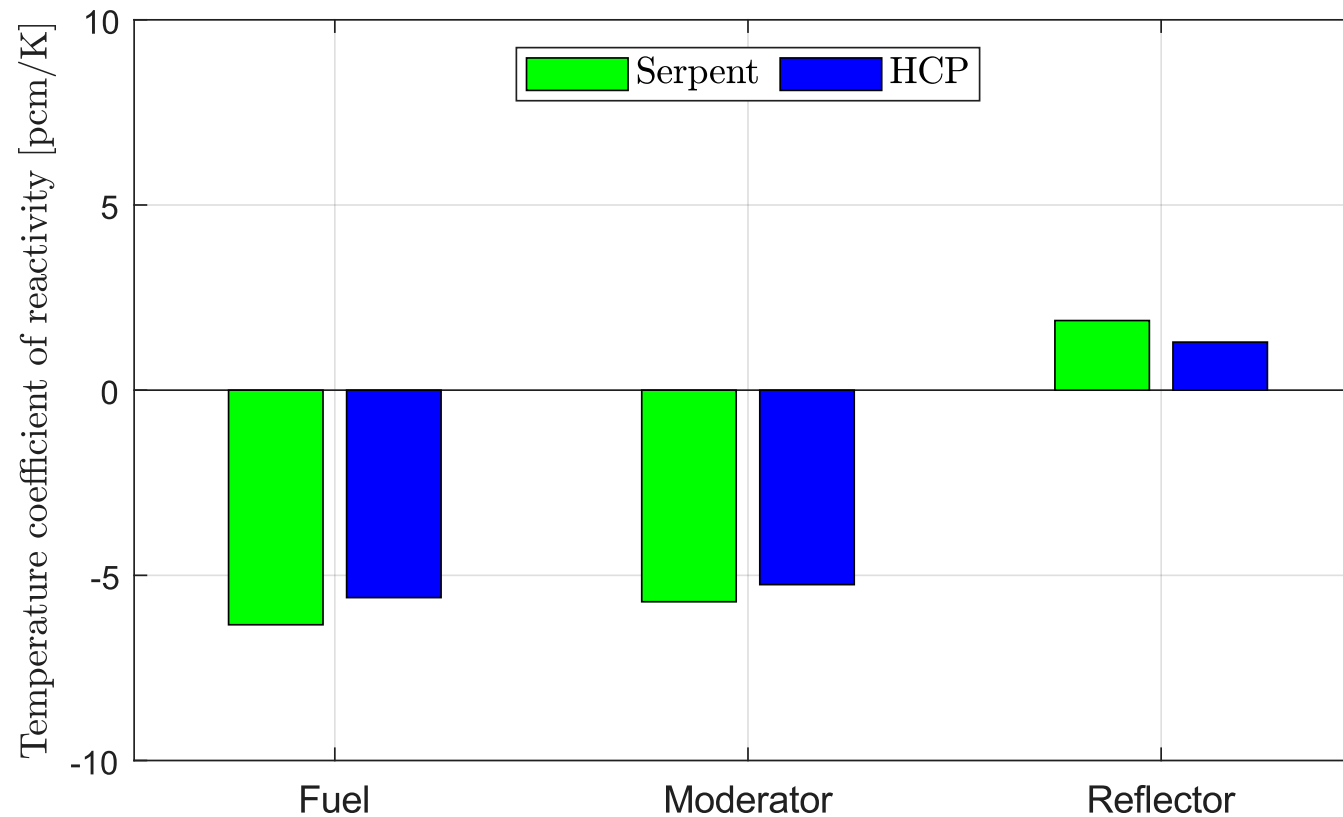
Core geometry of the HTR-PM model in the HCP:



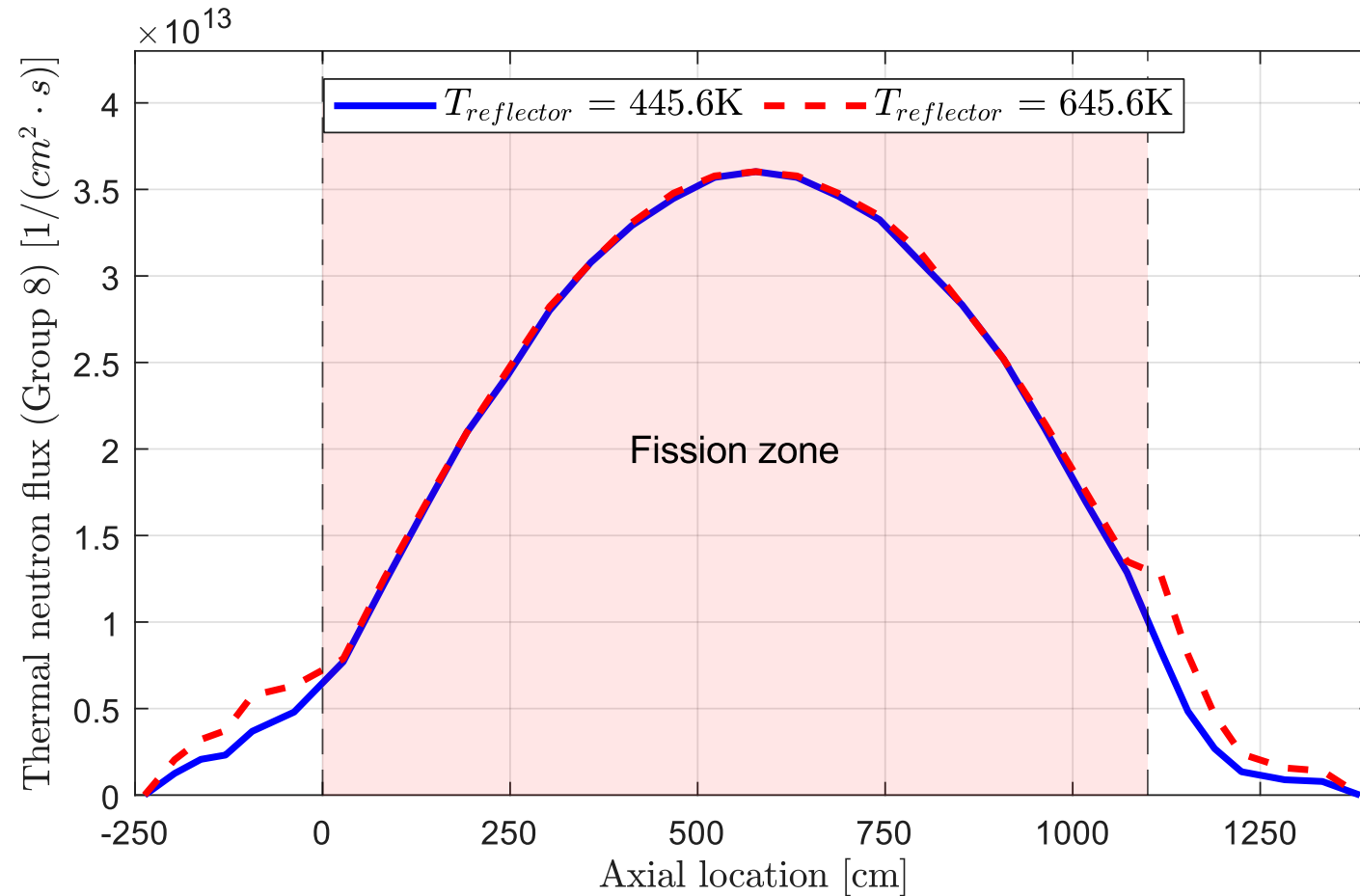
Comparison of power distribution:
(a) HCP results vs. (b) Serpent results



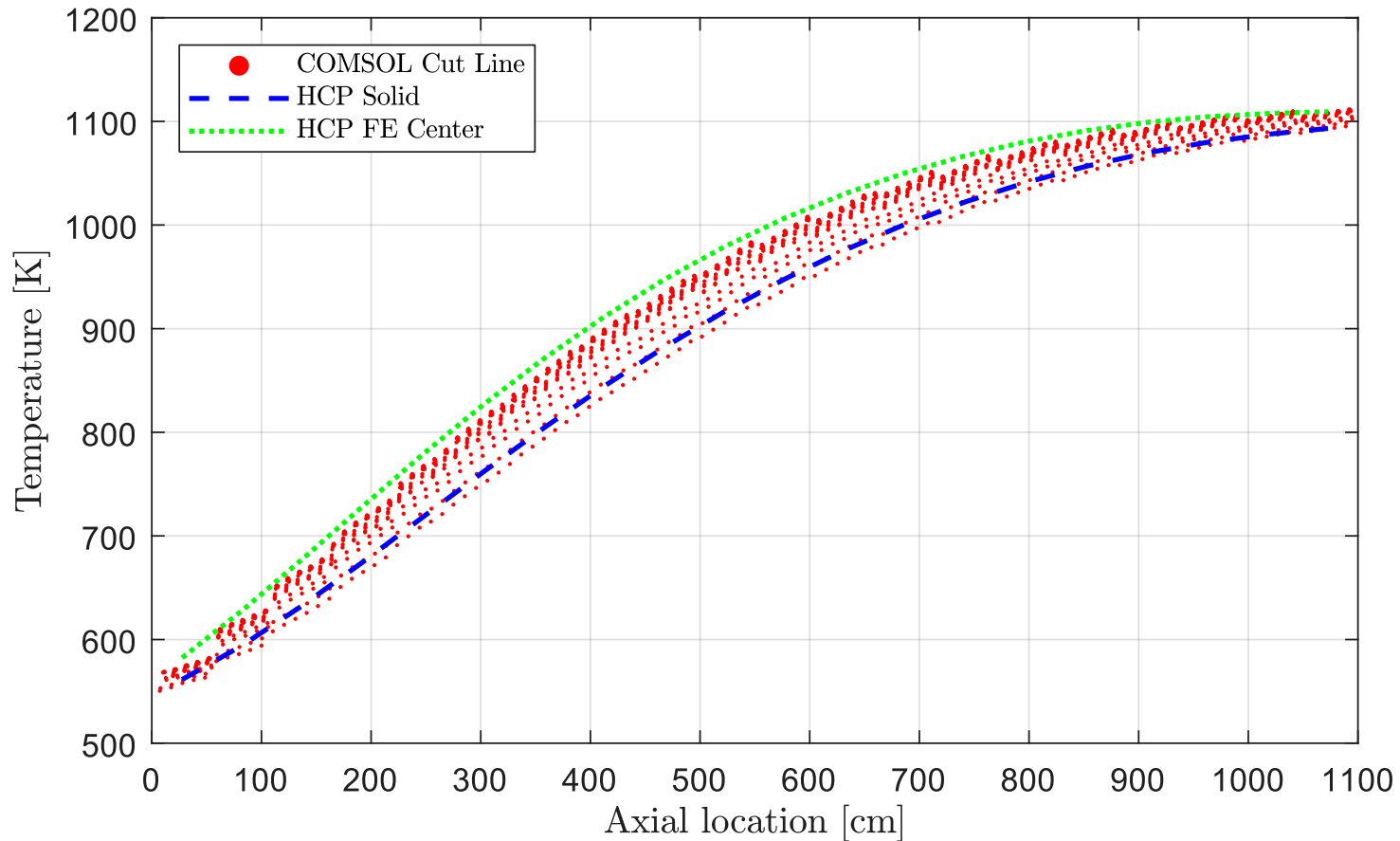
Comparisons of temperature coefficients of reactivity:
fuel, moderator and reflector



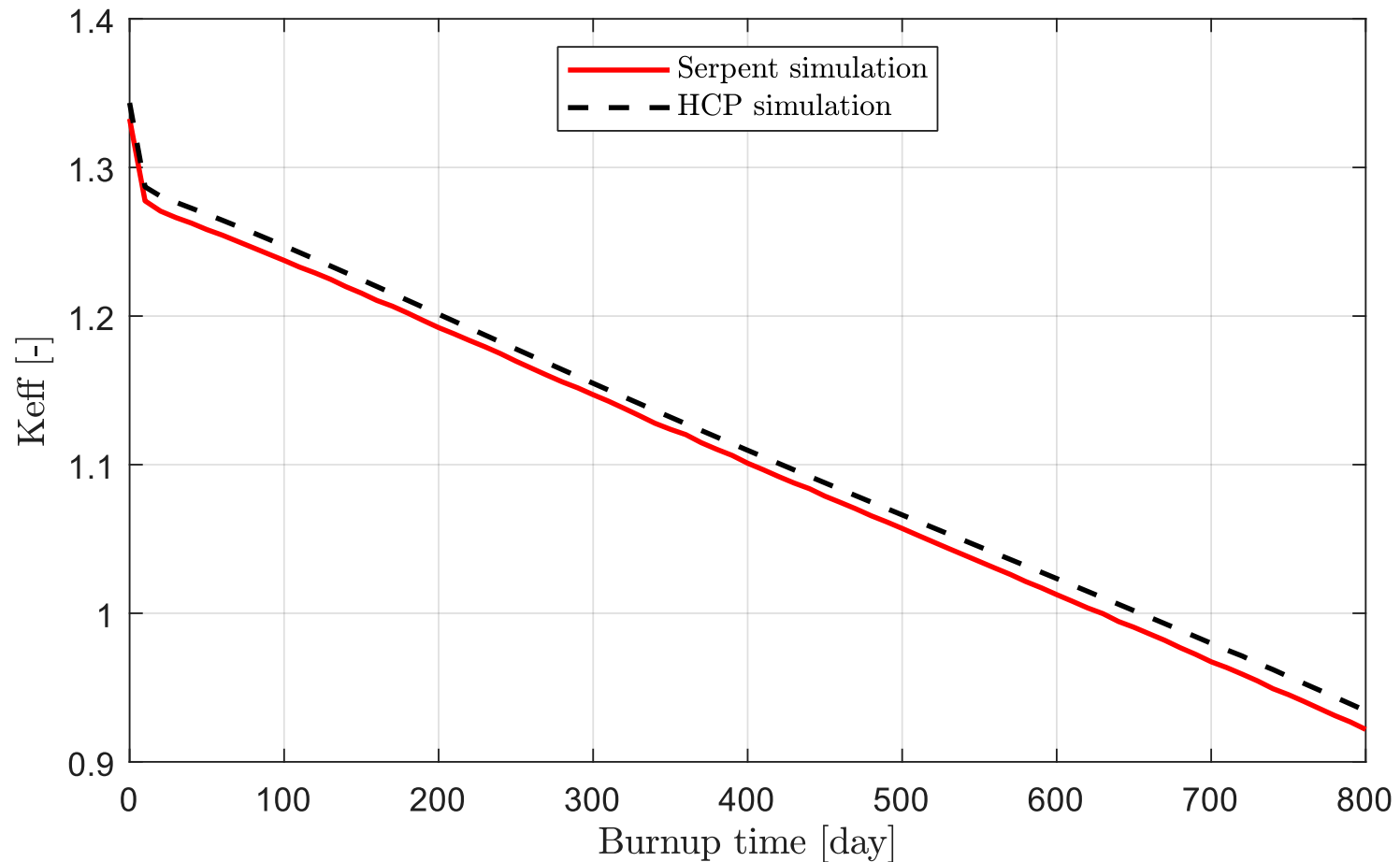
Neutron flux distribution at different reflector temperatures



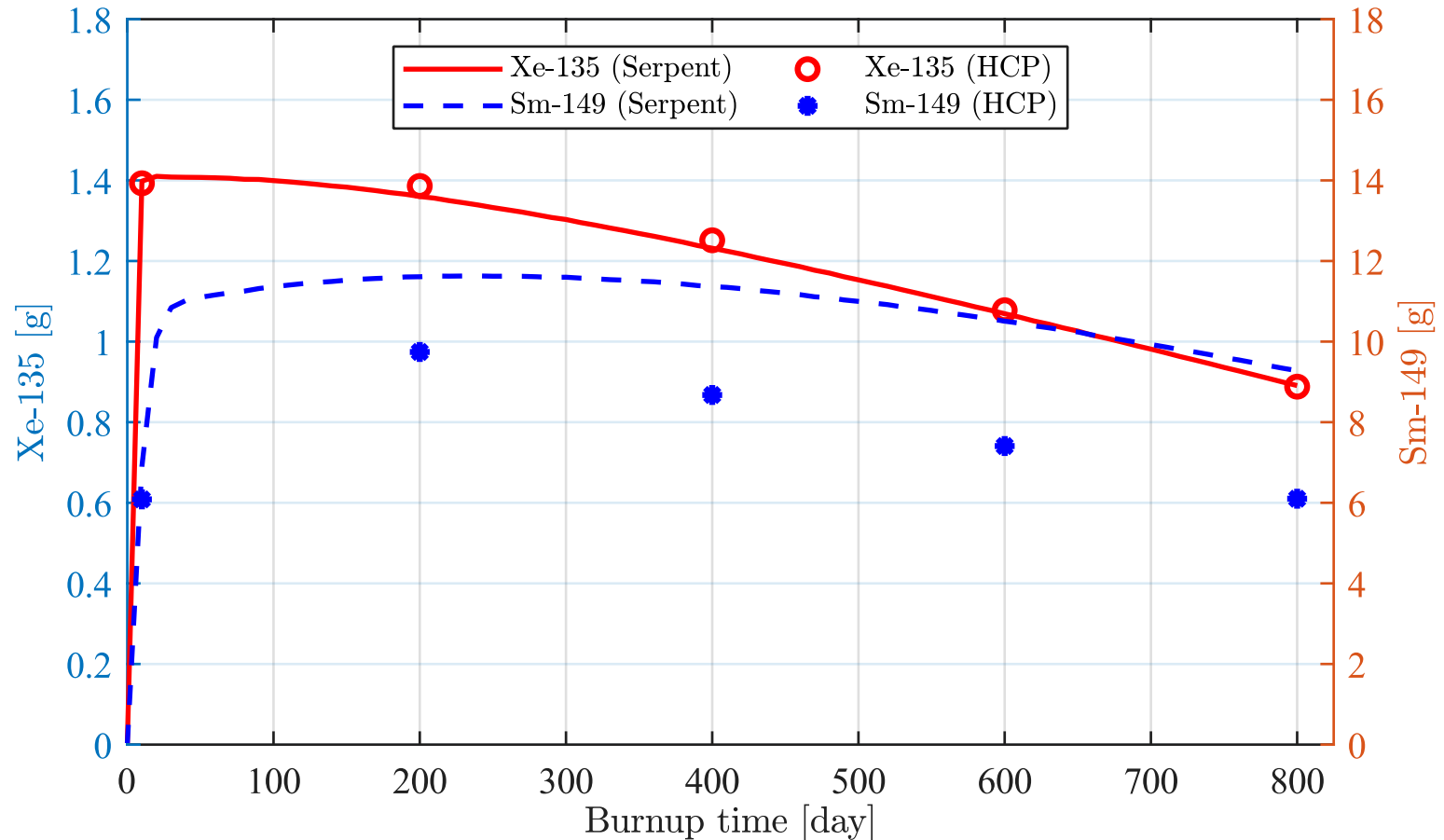
Comparison of solid temperature distributions in the hot channel



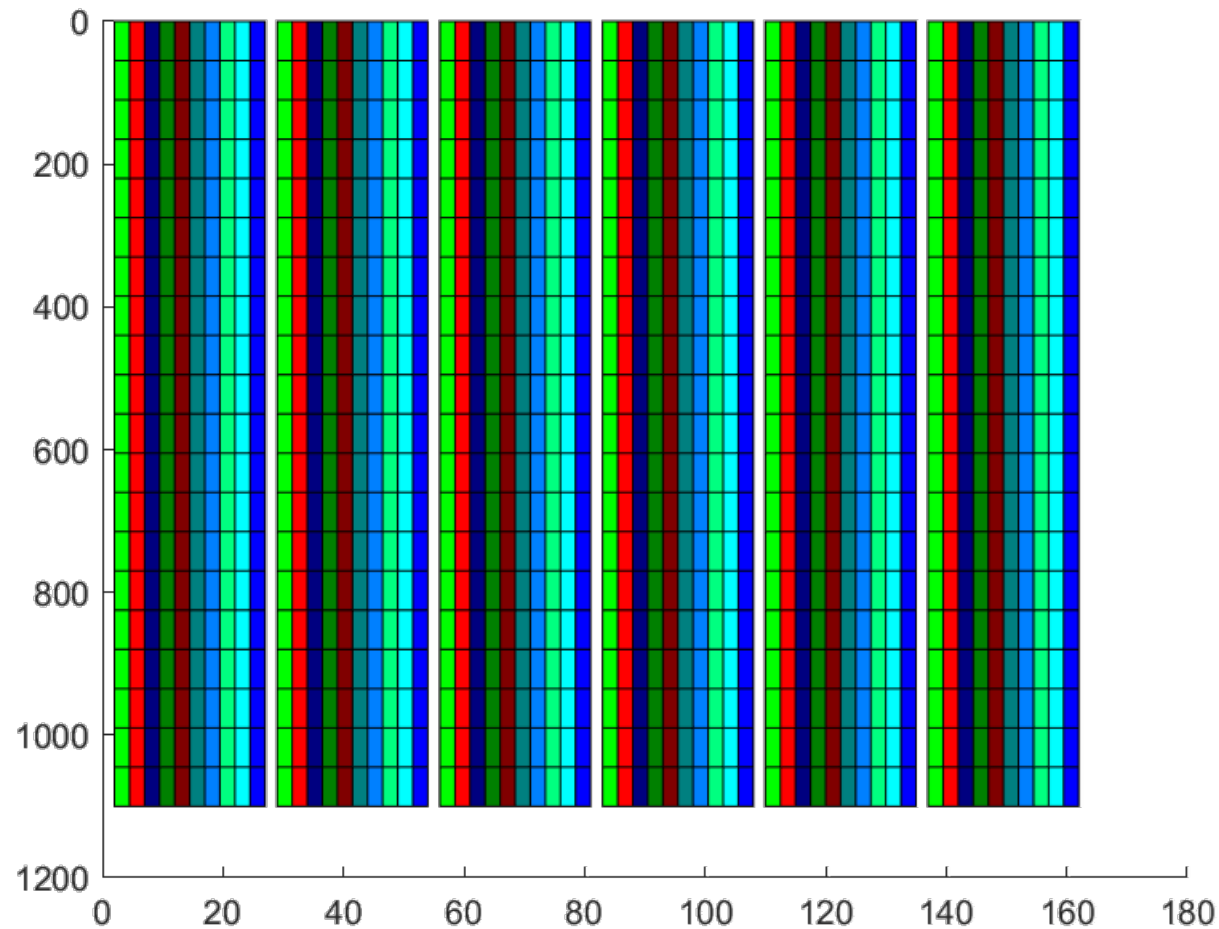
Evolution of k_{eff} during an 800-day burnup period



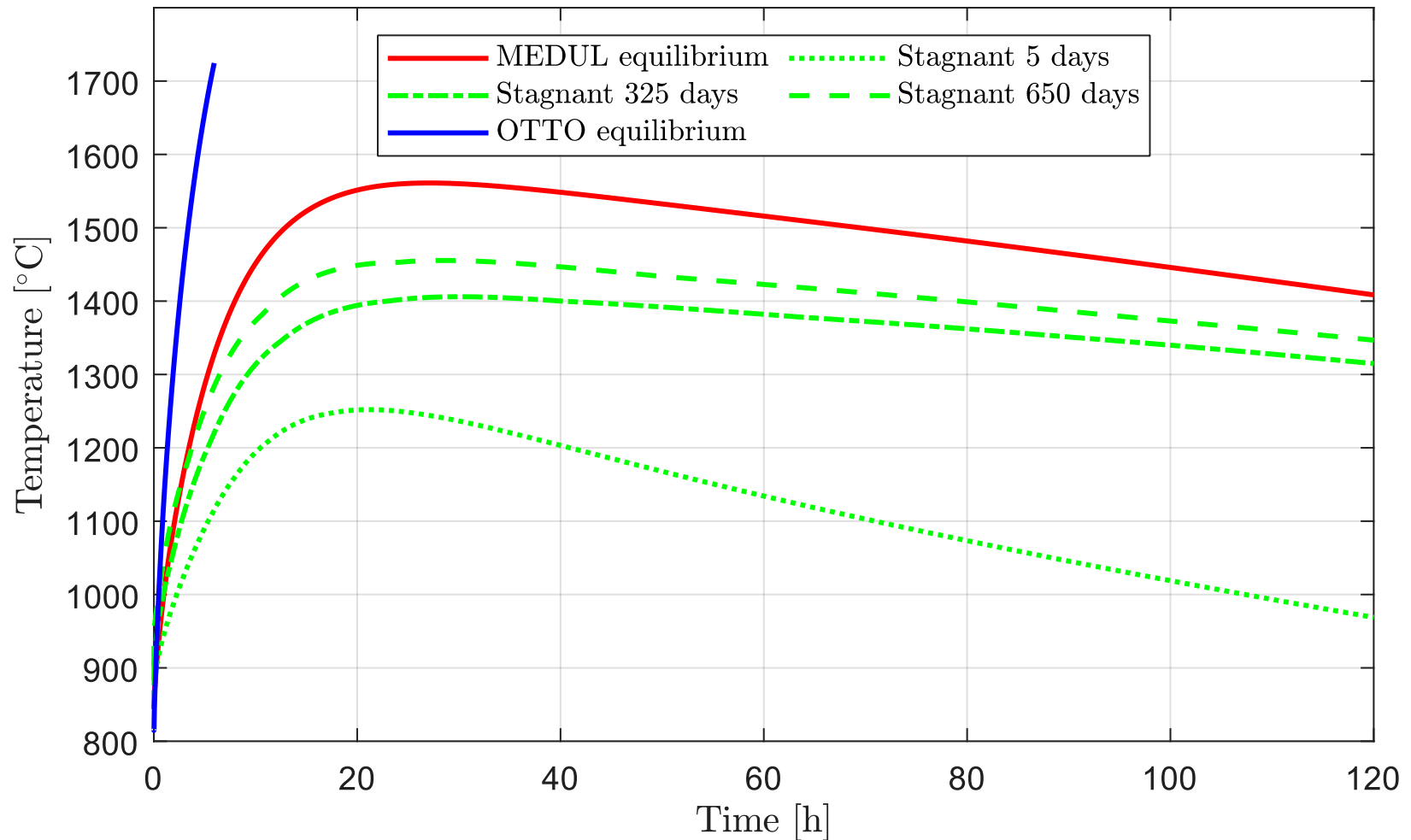
Mass evolution of poisonous fission products (Xe and Sm) during an 800-day burnup period.



Equilibrium core with 1200 batches

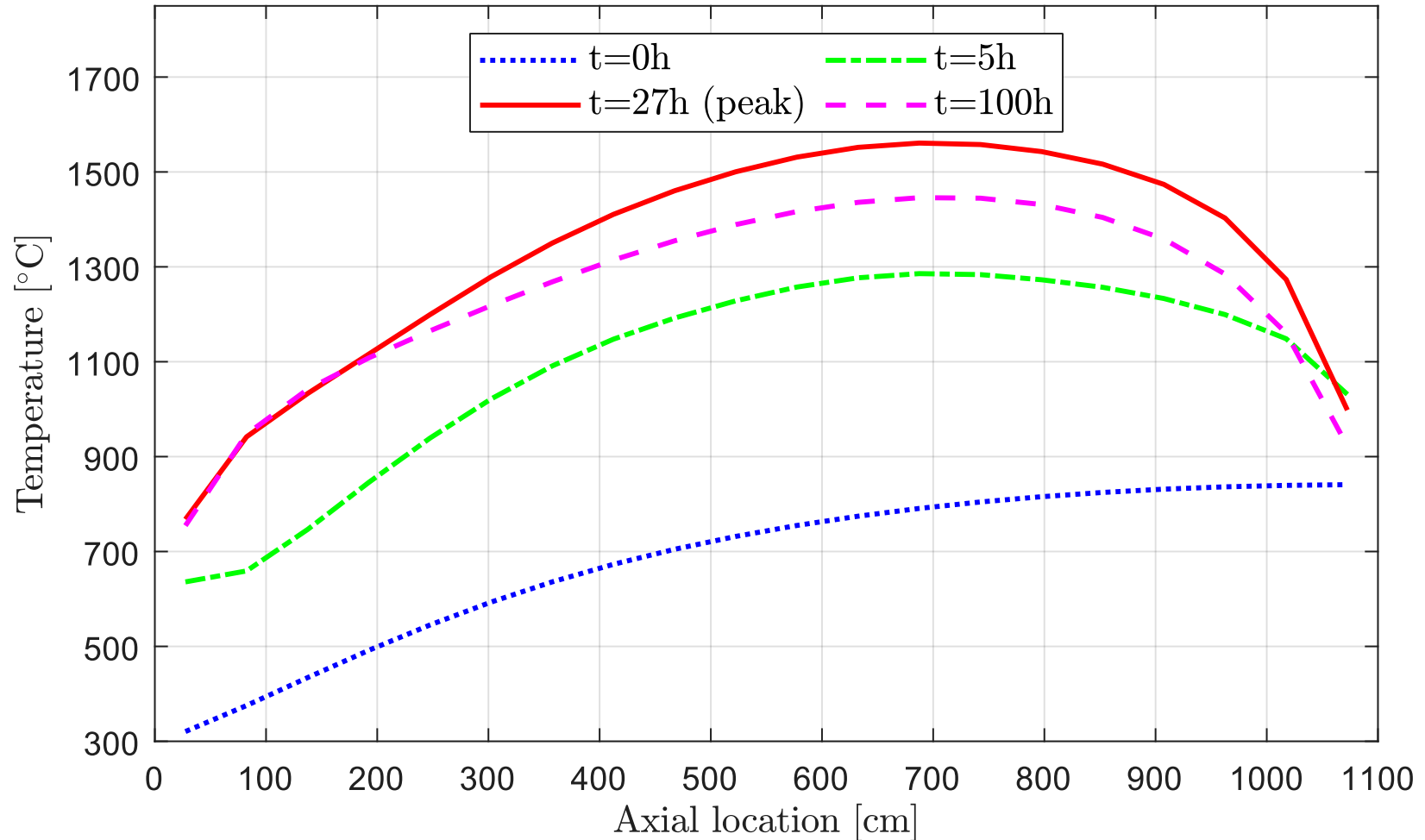


Peak of the fuel temperature during the DLOFC transient



With the MEDUL equilibrium core:

Fuel temperature distribution during the DLOFC transient



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Working Directory

..		2/14/2024 06:21:55	rw-rwxr-x	ntecher
data.p2d	90 KB	8/27/2024 00:48:00	rw-rw-r--	ntecher
data.pnd	85 KB	8/27/2024 00:48:00	rw-rw-r--	ntecher
data.ptr	0 KB	1/30/2024 02:32:25	rw-rw-r--	ntecher
data.rtn	0 KB	1/30/2024 02:32:25	rw-rw-r--	ntecher
DataSet.xml	1 KB	1/25/2024 09:07:59	rw-rw-r--	ntecher
Model.xml	50 KB	8/26/2024 23:07:15	rw-rw-r--	ntecher
output.txt	482 KB	8/27/2024 00:48:00	rw-rw-r--	ntecher
rstrt11.rtn	1,709 KB	8/27/2024 00:48:00	rw-rw-r--	ntecher
Scenario.xml	7 KB	1/28/2024 08:25:52	rw-rw-r--	ntecher
tispec.txt	0 KB	1/30/2024 02:32:25	rw-rw-r--	ntecher

DataSet.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<DataSet xmlns="http://www.example.org/DataSet"
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:schemaLocation="http://www.example.org/DataSet ../../../../xmlschemas/DataSet.xsd">

  <Header>
    <Title> HTR-PM Fresh Fuel Steady-State </Title>
    <Info>
      HTR-PM Model with Fresh Fuel.
    </Info>
    <Date> 2024-01-17 </Date>
    <Users n="1">
      <User>
        <LastName> Liu </LastName>
        <FirstName> Chunyu </FirstName>
        <Mail> chunyu.liu@tum.de;luoponan@gmail.com </Mail>
        <Org> TUM </Org>
      </User>
    </Users>
  </Header>

  <Paths>
    <DataLibrary inputType="binary"> ../../../../libs/Linux/endfb70_regtest_new.bin </DataLibrary>
    <Scenario> Scenario.xml </Scenario>
    <Model> Model.xml </Model>
    <SpecLib> ../../../../libs/SPECLIBN2009.lib</SpecLib>
  </Paths>
</DataSet>
```

Scenario.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<Scenario xmlns="http://www.example.org/Scenario"
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:schemaLocation="http://www.example.org/Scenario ../../../../xmlschemas/Scenario.xsd ">

  <Header>
    <Title> HTR-PM Fresh Fuel Steady-State </Title>
    <Info>
      HTR-PM Model with Fresh Fuel.
    </Info>
    <Date> 2024-01-17 </Date>
    <Users n="1">
      <User>
        <LastName> Liu </LastName>
        <FirstName> Chunyu </FirstName>
        <Mail> chunyu.liu@tum.de;luoponan@gmail.com </Mail>
        <Org> TUM </Org>
      </User>
    </Users>
  </Header>

  <Preferences scope="default">
    <Settings type="General">
    </Settings>
    <Settings type="Burnup">
    </Settings>
    <Settings type="Special">
    </Settings>
    <Settings type="FluidDynamics">
    </Settings>
    <Settings type="Neutronics">
    </Settings>
    <Settings type="Spectrum">
    </Settings>
  </Preferences>

  <DataInput scope="default">
  </DataInput>
  <DataOutput scope="default">
  </DataOutput>
  <TimeLine nActions="1">
  </TimeLine>
</Scenario>
```

Model.xml

```
<?xml version="1.0" encoding="UTF-8" standalone="no" ?>
<Model xmlns="http://www.example.org/Model"
  xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
  xsi:schemaLocation="http://www.example.org/Model ../../../../xmlschemas/Model.xsd">

  <Header>
    <Title> HTR-PM Fresh Fuel Steady-State </Title>
    <Info>
      HTR-PM Model with Fresh Fuel.
    </Info>
    <Date> 2024-01-17 </Date>
    <Users n="1">
      <User>
        <LastName> Liu </LastName>
        <FirstName> Chunyu </FirstName>
        <Mail> chunyu.liu@tum.de;luoponan@gmail.com </Mail>
        <Org> TUM </Org>
      </User>
    </Users>
  </Header>

  <FuelCollections n="1">

    <!-- Only non default values are given!-->
    <Components>

    <FuelElements n="1">

    <ParticleCompositions n="1">

    <Particles n="1">

    <Materials n="5">

    <GeoObjects n="8">
  </Model>
```

Running the Simulation

```
ntecher@NTechPC: ~  
ntecher@NTechPC:~$ runproto ../../data/input/2024b_HCP/HTRPM_test04_861/DataSet.xml
```

```

EQUILIBRIUM CALCULATION(%-INFORM. WITH RESPECT TO EQUILIBRIUM POWER 2.5000D+08 W)
  CPUS IFG  VFT IGS  VGT DP21  P  TK1 TK2 TK3  MP1 WQK  BZTM  VNL  WQNT  KEFF
  (S)      ITF (K)  IMX (K) (MB) (B) (C) (C) (C) (KG/S) (%) (C)  ITN  (%)  (%)
10      1.34 100.11 1.33210890612
10     -0.24 100.02 1.33745538719

Running fluid dynamics calculation...
The steady state temperature in the choosen fuel element mesh grid
yields an error of -0.101 degrees centigrade

12. 20 28 342.1 56 0 345.161949. 70.0 737. 250. 259.-9.60D+01 97.17 891.
Running nuclear calculation...
10 -0.29 100.01 1.32619245008
10 -0.08 100.00 1.32663894033

Running fluid dynamics calculation...
22. 20 24 102.9100 0 102.9 948. 70.0 751. 250. 263.-9.60D+01 99.93 887.
Running nuclear calculation...
10 0.04 100.00 1.32290395890
10 0.02 100.00 1.32286740980

Running fluid dynamics calculation...
32. 20 20 8.4100 0 -9.9 952. 70.0 751. 250. 264.-9.60D+01 99.93 885.
Running nuclear calculation...
10 0.01 100.00 1.32235581402
10 0.00 100.00 1.32234769240

Running fluid dynamics calculation...
45. 20 20 -2.1 98 0 -6.1 953. 70.0 751. 250. 264.-9.60D+01 99.93 885.
Running nuclear calculation...
10 0.00 100.00 1.32222713235
10 0.00 100.00 1.32222469795

Running fluid dynamics calculation...
55. 20 20 -1.4 97 0 -4.4 953. 70.0 751. 250. 264.-9.60D+01 99.93 885.
Running nuclear calculation...
10 0.00 100.00 1.32219070415
10 0.00 100.00 1.32218996734

Running fluid dynamics calculation...
67. 20 20 -0.9 97 0 -2.9 953. 70.0 751. 250. 264.-9.60D+01 99.93 885.
Running nuclear calculation...

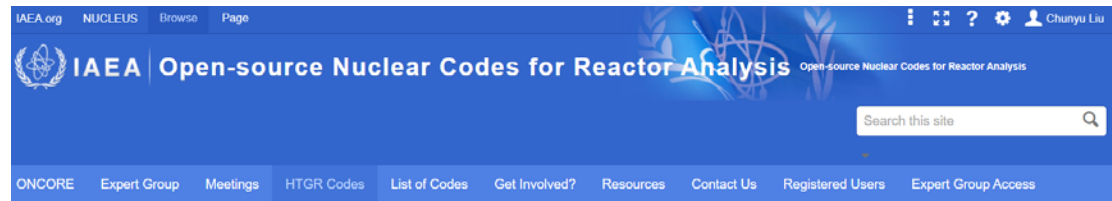
```

Simulation Finished

```
ntecher@NTechPC: ~  
Model 1 contains at least one node (id = 100) holding batch 100 holding 12 nuclides.  
1 | 922350 | amount = 13.6482 mole  
2 | 80160 | amount = 316.652 mole  
3 | 80170 | amount = 0.120621 mole  
4 | 80180 | amount = 0.650717 mole  
5 | 140280 | amount = 328.05 mole  
6 | 140290 | amount = 16.6652 mole  
7 | 922380 | amount = 145.063 mole  
8 | 140300 | amount = 10.9987 mole  
9 | 60120 | amount = 84202.1 mole  
10 | 50110 | amount = 0.0892327 mole  
11 | 60130 | amount = 1022.7 mole  
12 | 50100 | amount = 0.0221689 mole  
Model 1 contains at least one node (id = 120) holding batch 120 holding 12 nuclides.  
1 | 922350 | amount = 16.6811 mole  
2 | 80160 | amount = 387.019 mole  
3 | 80170 | amount = 0.147425 mole  
4 | 80180 | amount = 0.795321 mole  
5 | 140280 | amount = 400.95 mole  
6 | 140290 | amount = 20.3686 mole  
7 | 922380 | amount = 177.299 mole  
8 | 140300 | amount = 13.4428 mole  
9 | 60120 | amount = 102914 mole  
10 | 50110 | amount = 0.109062 mole  
11 | 60130 | amount = 1249.96 mole  
12 | 50100 | amount = 0.0270953 mole  
  
*****  
  
*****  
11:58:07 | INFO | HCP-MAIN > main  
*****  
  
run finished on Wednesday, 09/24/25, 11:58:07 AM  
ntecher@NTechPC:~$
```

Software request via IAEA:

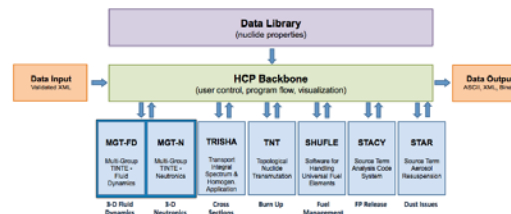
<https://nucleus.iaea.org/sites/oncore/htgr-codes/SitePages/HCP.aspx>



Home
Download Codes
VSOP
STACY
HCP
Discussion Forums
VSOP Forum
STACY Forum
HCP Forum
Expert Group
Pages

HCP

HCP (HTR Code Package)



The HTR code package (HCP) allows for the simulation of several safety-related aspects of a High Temperature Reactor core in a highly integrated manner. The main objective of the code is the "Design, implementation and validation of software for the simulation of V/HTRs by applying the latest programming techniques and standards". HCP has full three-dimensional capabilities. This is not available in any other integrated HTR code system, especially not for pebble bed reactors. HCP replaces all the old legacy codes developed at the Research Centre Juelich over more than 40 years from the 1970's until 2010. Development continued (several PhD studies till ~2019).

NOW AVAILABLE FOR RELEASE:
(two main research versions that historically existed have been harmonised and a single version is now available that run a larger selection of test cases. The code will be further developed and those interested to test or develop the code can get access to the source code and participate in ONCORE initiatives to enhance the code)

Contact the IAEA if you want to have access to the source code and also contribute to the hcp development:

oncore@iaea.org

[Download Executable \(with sample I/O\)](#)

[Download Installation Instructions, Video](#)

HCP User Forum:

<https://nucleus.iaea.org/sites/oncore/htgr-codes/Lists/HCP%20Discussion%20Forum/AllItems.aspx>

Contacts

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Overview

- Introduction of the HTR Code Package (HCP)
- Progress in the research project KONHCP I
 - Implementation of control rod
 - IT work
- Outlook for the research project KONHCP II
 - Implementation of molten salt coolant
 - Implementation of prismatic geometry
 - Further integration of the STACY module
- Advances in Independent Research
 - Conductive heat transfer calculation
 - LibGen fixing and I/O improvement
 - Benchmark and safety analysis
- HCP Demonstration, Application, and User Forum
- **Summary**

- **Outcome:**

- 2 PhD dissertations
- 3 journal papers, 2 conference papers
- 2 training courses organized by IAEA
- 2 batches of on-site training programs
- International collaborations

- **To be done:**

- KONHCP I deliverable: new code version with manual, release notes, project report
- Update of the HCP version on ONCORE
- KONHCP II
- General coupling interface
- External components/loops

Thanks!