LA-UR-17-28187

Demonstration of Multi-physics calculation for accelerator-driven LEU solution technology for Mo^{99}

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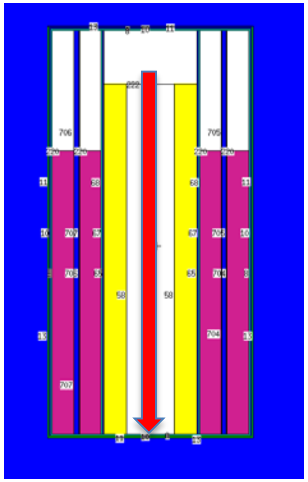
Table of contents

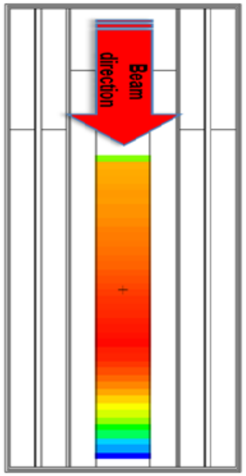
1. Background & motivation
   - Accelerator driven fissile solution technology
   - Multiphysics coupled calculation
2. Neutronic + Thermal Hydraulic solver
   - MCNP
   - Multiphase CFD
3. CASE study
   - Base case (CASE1) coupled calculation
   - 4 different neutron source cases
4. Incremental methodology development
   - Method-1 : Single-cell approach + constant solution height
   - Method-2 : Single-cell approach + dynamic height adjustment
   - Method-3 : Multi-cell approach + dynamic height adjustment
5. Summary and Future works

Accelerator driven fissile solution system for Mo99

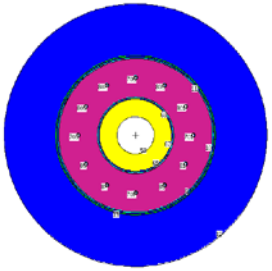
Fissile Solution Vessel model in MCNP

Side view





Top view



Fissile Solution Vessel → pink
Moderator → Yellow
Light water → blue
Vacuum → White
Zircaloy4 → Turquoise

System design features

- 12 cooling tubes
- OD of FSV = 0.70m
- Height of FSV =1.053m
- Height of moderator = 1.3m
- Initial Solution Volume = 300L

Background:

- ❑ *Mo99 is a critical isotope in medical applications*
- ❑ *Domestic Mo99 needs are demanding (No production in USA)*

Innovations:

- ❑ *LEU based Mo99 production (No proliferation risk)*
- ❑ *Accelerator driven neutron source (subcritical, easy to turn off)*
- ❑ *Self-regulating feature (Liquid fuel reactor concept)*

Challenges:

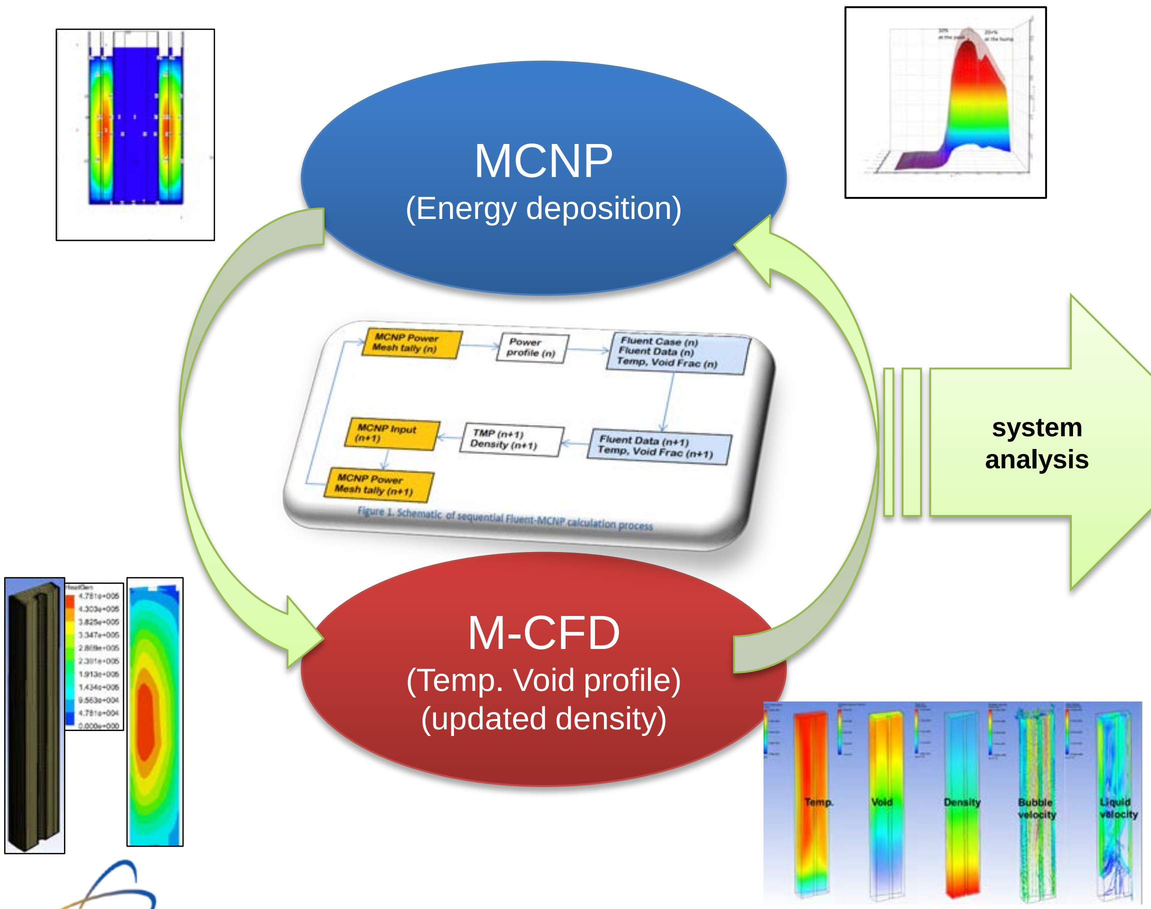
- ❑ ***Multi-physics coupled calculation for system evaluation***
- ❑ ***Bubbly flow modeling in TH code (i.e. Radiolytic gas)***
- ❑ ***Fissile Solution height adjustment (temp, void)***
- ❑ ***Non-uniform Fissile solution density***

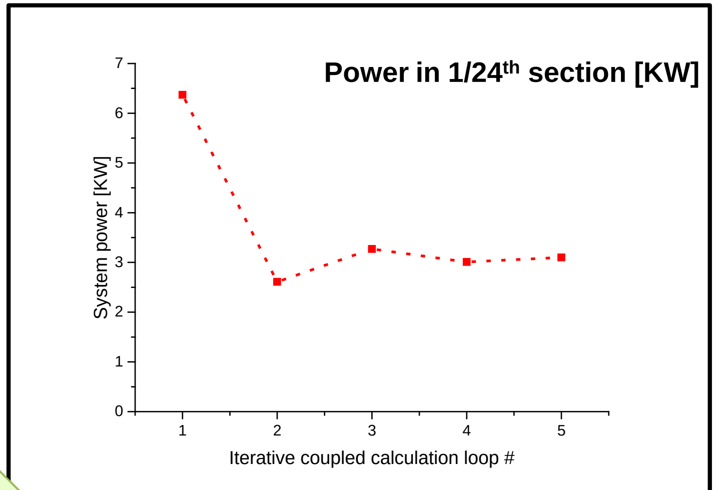
Applied simulation tools

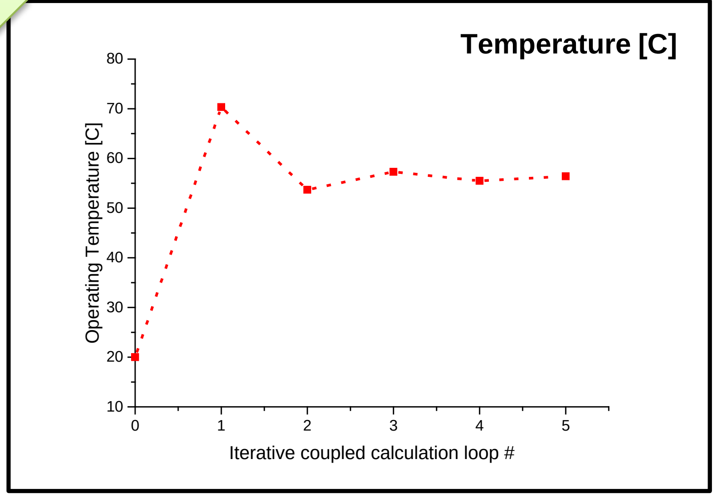
- ❑ *Neutronic calculation : MCNP6.2*
- ❑ *Thermal Hydraulic calculation : Fluent 17.2*
- ❑ *Automated coupling calculation frame toolkit : Python*
- ❑ *All calculation is performed in LANL HPC (Tebow and Pete)*

Multi-Physics modeling for fissile solution vessel

*(Power calculated by **MCNP** ←→ thermal hydraulic calculated by **M-CFD**)*

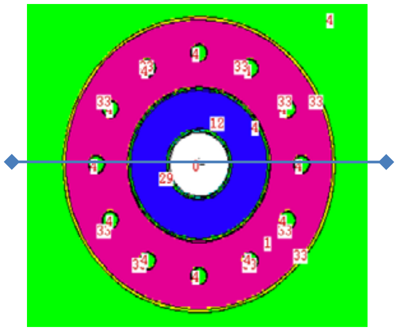


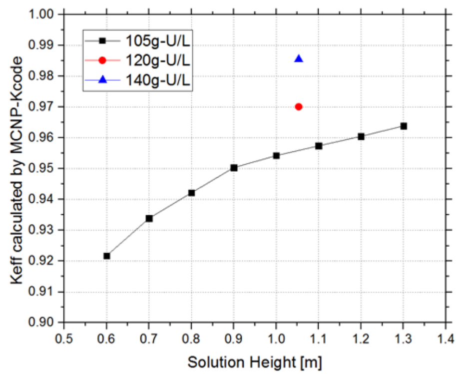




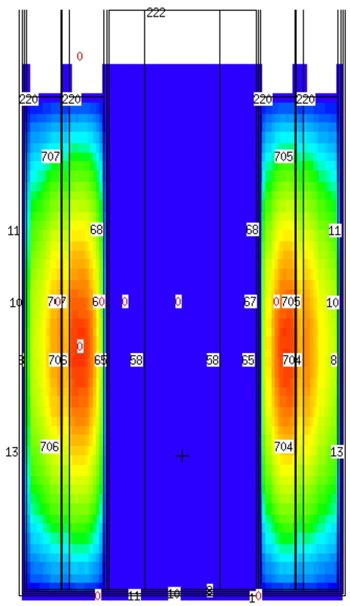
Neutronic solver (MCNP calculation)

Energy deposition calculation from heating tally in MCNP

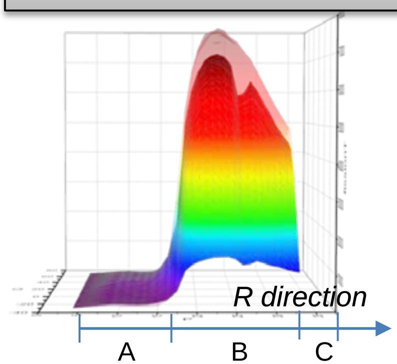




- *Energy deposition in vessel*
- *2D power profile (input for CFD)*



R direction



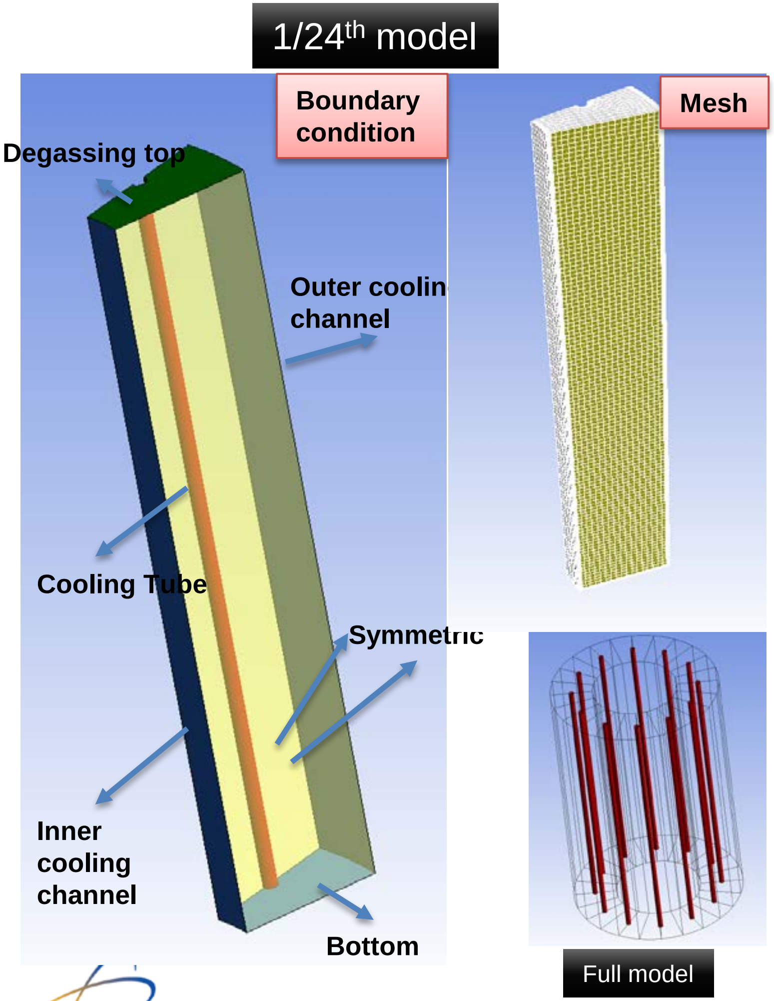
A: Vacuum + moderator zone (no heating)
B: Fissile solution zone (heating source)
C: Outer water pool (no heating)

Fissile solution vessel calculation

- MCNP6.2. used
- K-Code calculation is performed to evaluate the criticality of the system at the cold-start operating condition (Keff = 0.98)
- Reference solution for cold-start
  - Uranyl sulfate density : 1.85 kg/m3
  - Solution concentration : 140gU/L
  - Temperature : 20C
- Uranyl Sulfate aqueous solution
- Solution density is function of concentration & temperature
- Fission and heating tally are used to evaluate the azimuthally averaged power profile within the fissile solution vessel.

Thermal Hydraulic (Multiphase CFD calculation)

Temperature and void profile calculation in MCFD



Multiphase CFD specification

- Fluent17.2 used
- Eulerian based two fluid model approach
- Pseudo transient analysis for steady state calculation

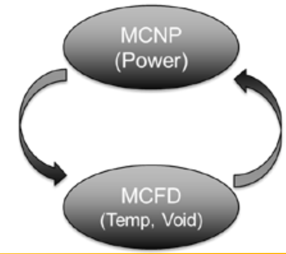
- Hex dominant mesh with prism mesh at the wall (Y+<1)
- URANS turbulence model (SST K-ω)

- Volumetric power (energy) and bubble generation (mass) profiles implemented by using UDF script
- Convergence check with residual variables and energy and mass balance
  - Energy in (MCNP) = Energy out (M-CFD)
  - Bubble generation = Bubble loss at degassing surface

- Convective heat transfer coefficients (HTCs) for outer side of cooling surfaces are evaluated based on empirical Gnielinski correlation.

- Multiphase closure model described in back-up slides

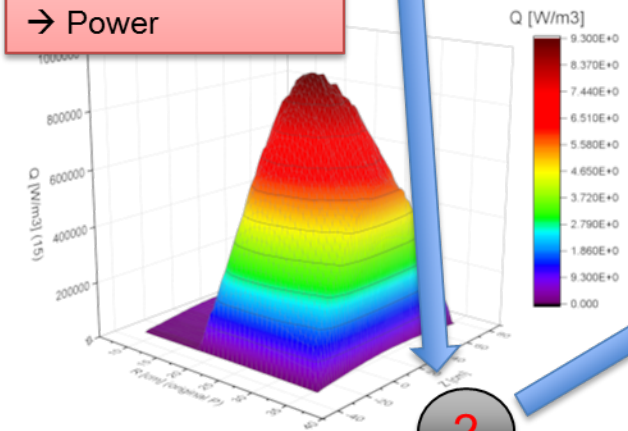
MCNP+MCFD Coupling procedures…



1

Cold start condition
20C, 1185.4 kg/m^3
(MCNP-run#1)

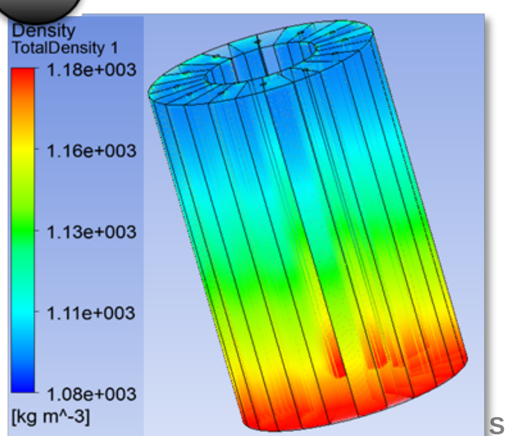
→ Power



2

Quasi st.st condition
(MCFD-run#1)

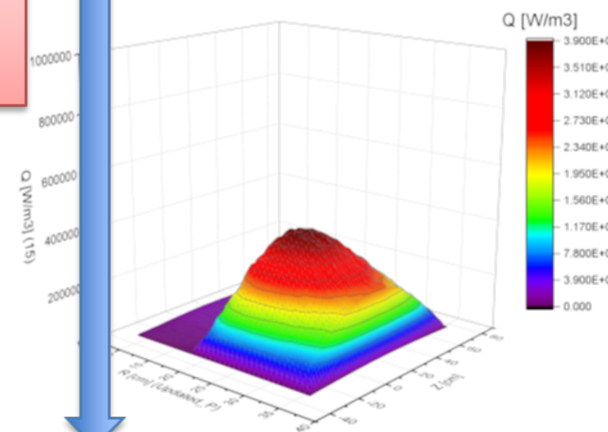
→Temp., Void, **Density**
(70.35C, 1128.6kg/m^3)



3

Updated condition
70.35C, 1128.6kg/m^3
(MCNP-run#2)

→ Updated power

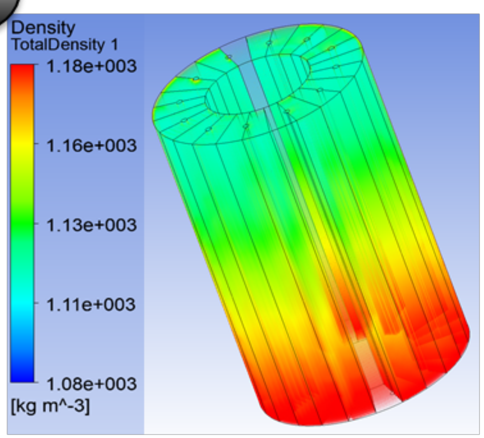


4

And continues…

Saturated condition
(MCFD-run#2)

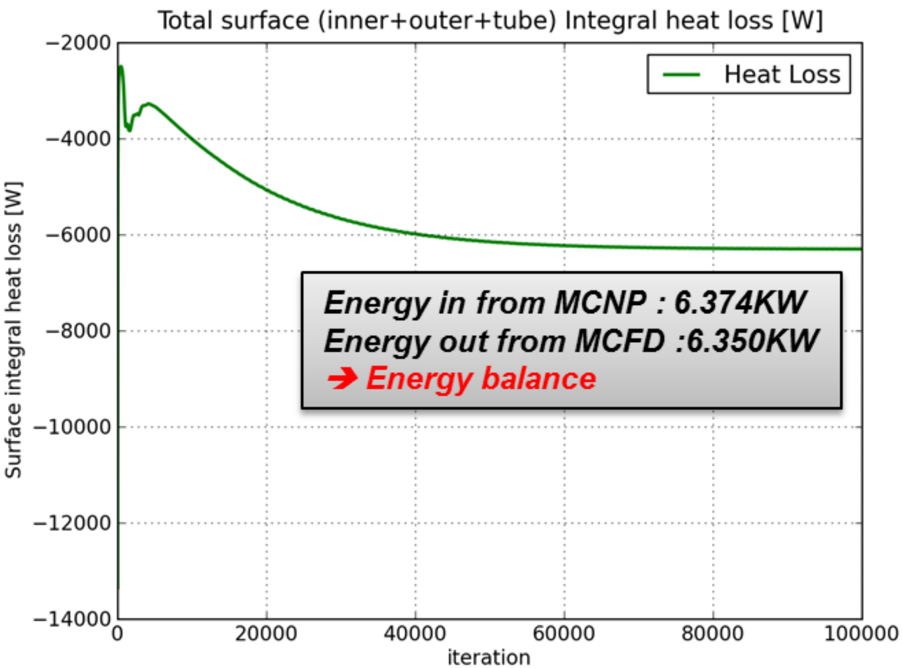
Updated density : :
53.7C, 1145.1kg/m^3

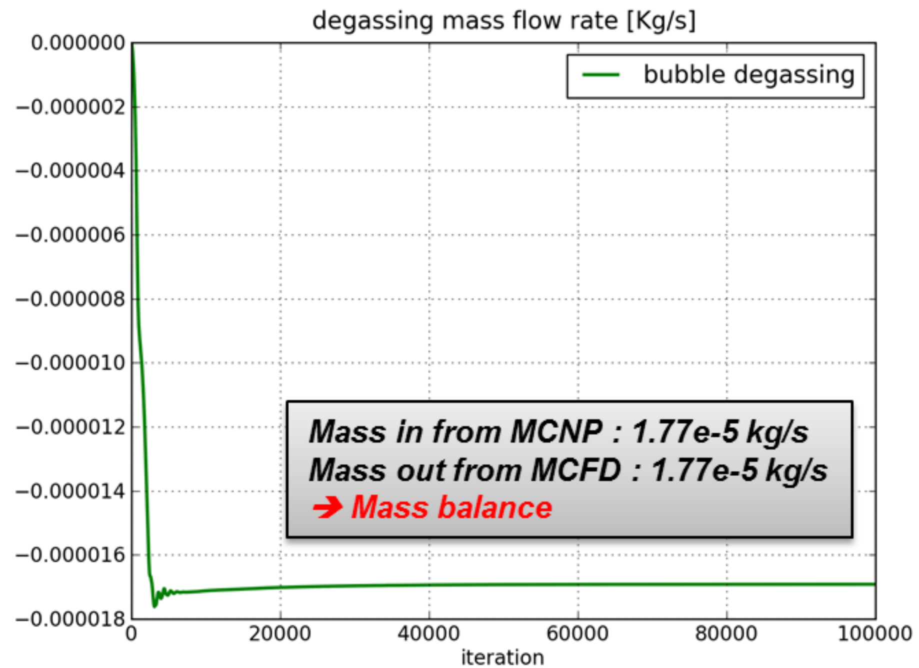


Convergence check in coupled calculation

Energy and mass balance between (MCNP & MCFD)

The CFD simulation converged with all N-S parameters residual less than 1e-4
In addition, Energy and mass balance are checked in every iterative calculations
For example. CASE-Run#1 (*Source neutron = 1.456e14 [s^{-1}]*)



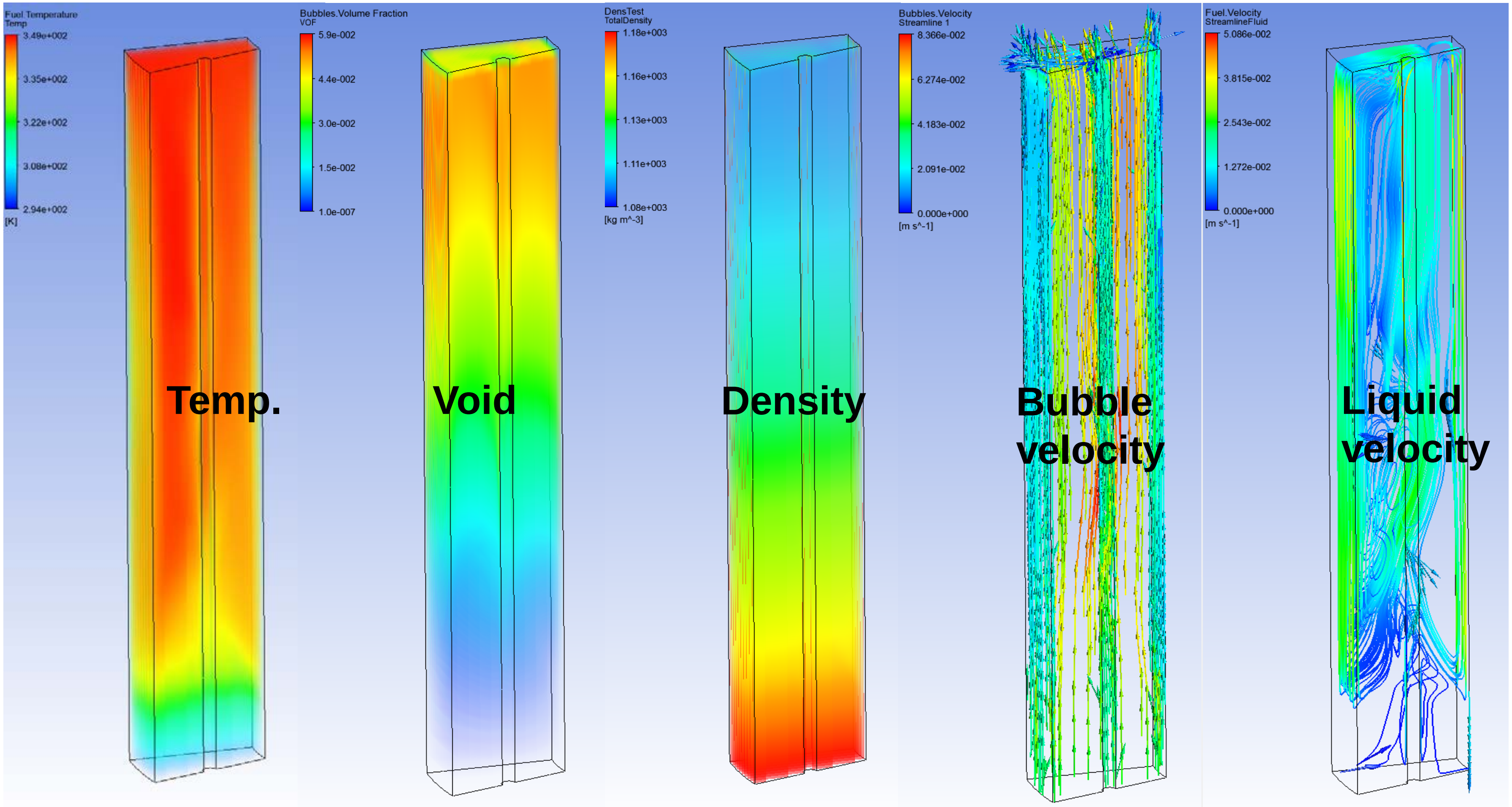


Energy out at the cooling surfaces

Mass out at the degassing surface

Thermal Hydraulic parameters calculated from M-CFD

Temp., Void distribution and bubble rising and liquid circulation pattern

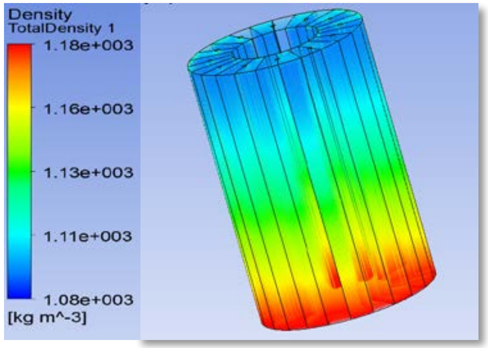


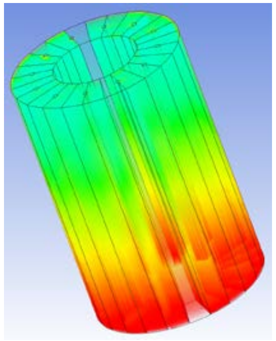
Preliminary results from CASE-run#1

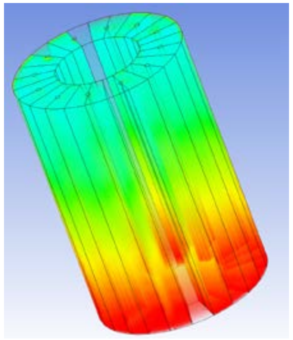
Summarized results from MCNP+MCFD calculation (I)

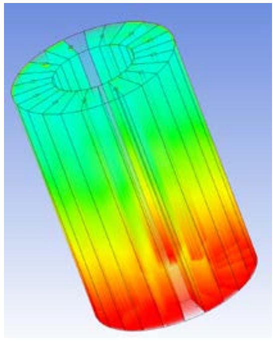
Operational parameters (system power, solution temp. & density) are saturated

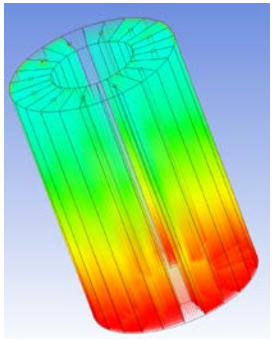
CASE-1 (SN=1.458e14s-1)	Run#1 (cold start)	Run#2	Run#3	Run#4	Run#5
MCNP ***Cold start condition*** ***(20C, 1185.4 kg/m3)***	Input: 20C, 1185.4 kg/m3 Output: 6.37KW	Input: MCFD-run#1 Output: 2.61KW	Input: MCFD-run#2 Output: 3.27KW	Input: MCFD-run#3 Output: 3.01 KW	Input: MCFD-run#4 Output: 3.10 KW
MCFD Predicted normal operating condition ***(56.4C, 1142.6kg/m^3)***	Input: MCNP-run#1 Output: 70.3C, 1128.6kg/m^3	Input: MCNP-run#2 Output: 53.7C, 1145.1kg/m^3	Input: MCNP-run#3 Output: 57.3C, 1141.8kg/m^3	Input: MCNP-run#4 Output: 55.9C, 1143.0kg/m^3	Input: MCNP-run#5 Output: 56.4C, 1142.6kg/m^3









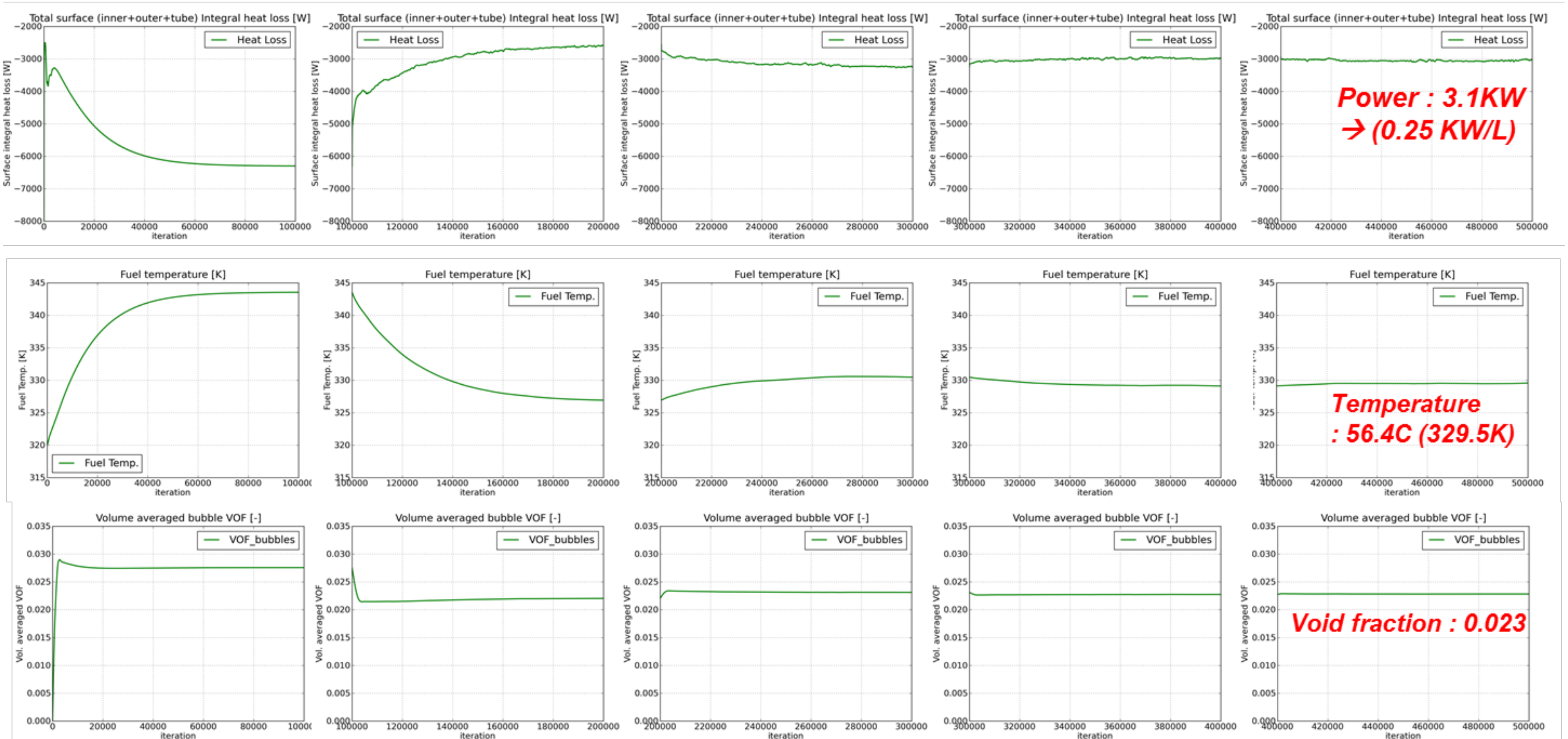


Solution density profile is saturated as coupled simulation is progressed

Summarized results from MCNP+MCFD calculation (II)

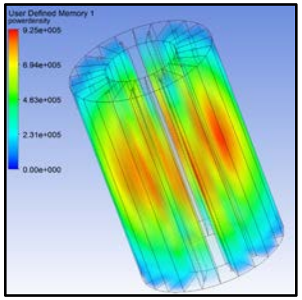
Operational parameters (system power, solution temp. & density) are saturated

MCFD-run#1 | MCFD-run#2 | MCFD-run#3 | MCFD-run#4 | MCFD-run#5



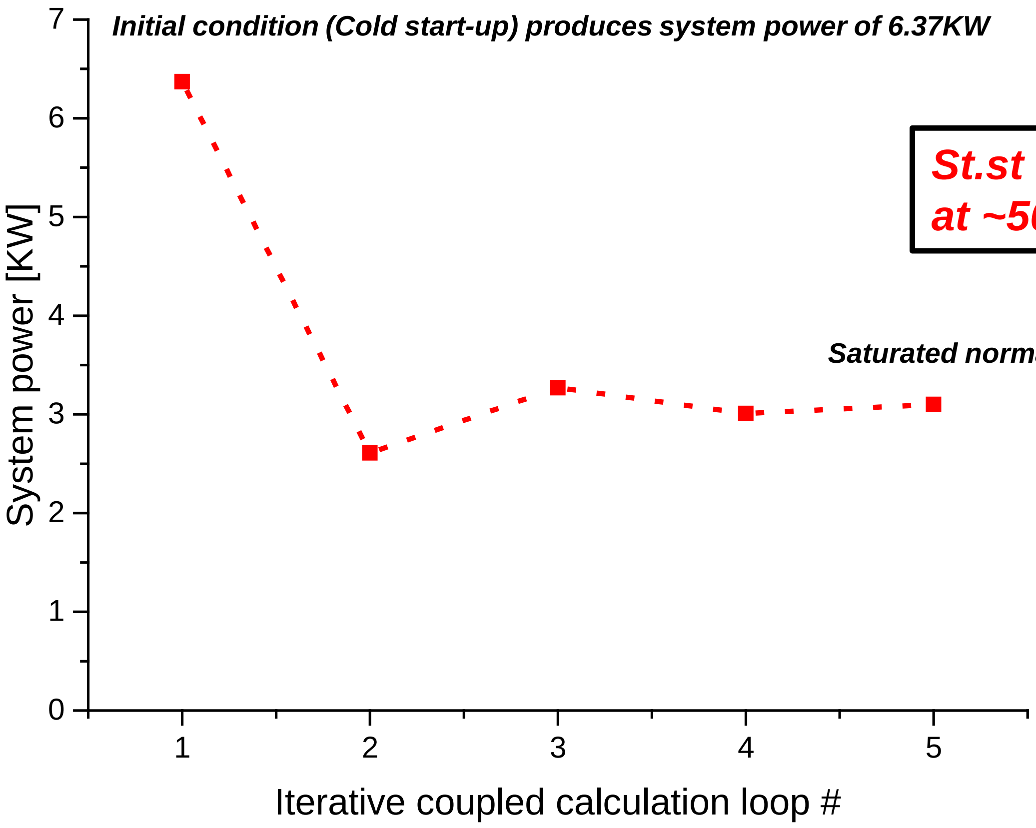
Prediction of operational system power at the steady state

(Converging to normal operating power)

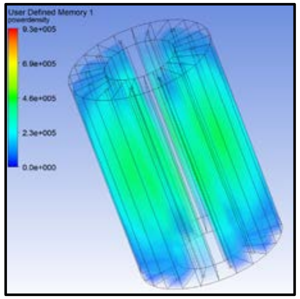


MCFD-run#1

CASE1 with initial SN=1.458e14s-1



St.st system power saturated at ~50% of cold-start level…

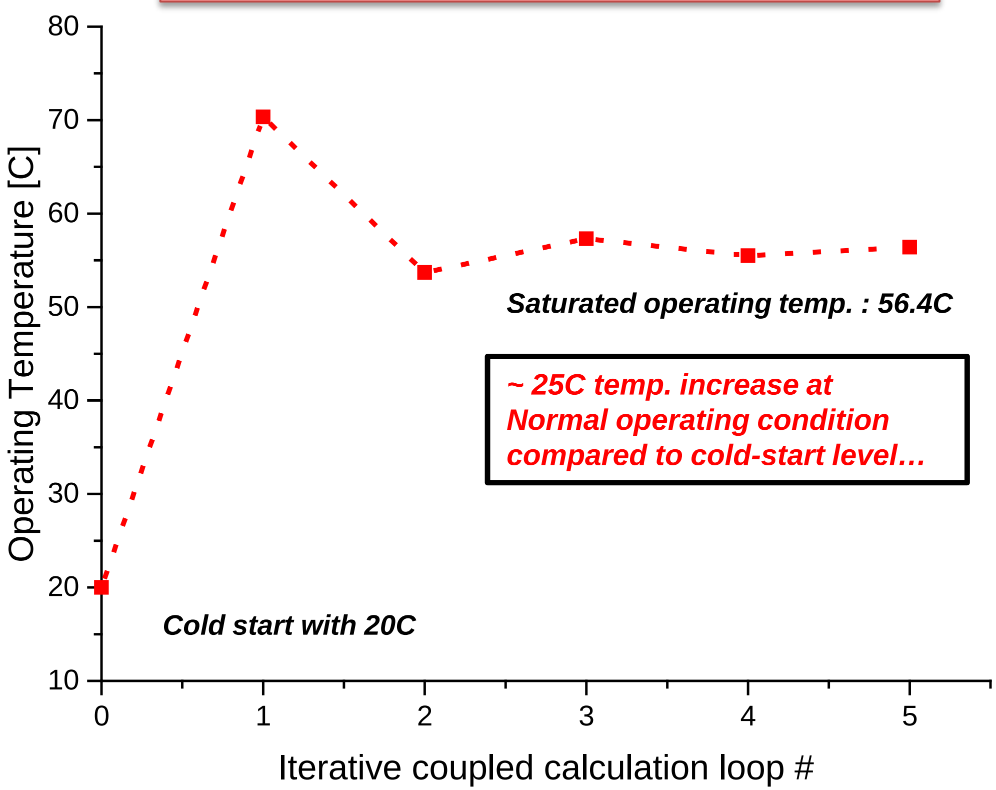


MCFD-run#5

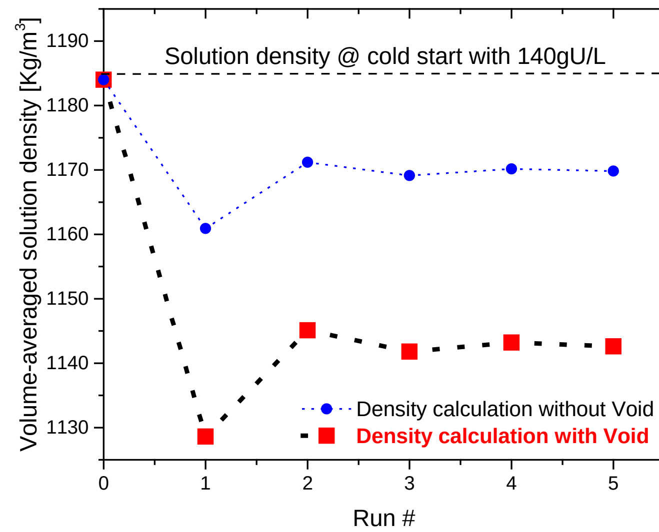
Prediction of operational solution thermal hydraulics

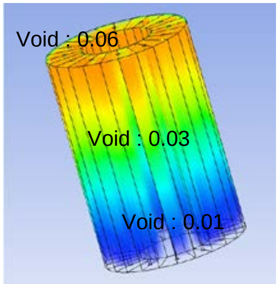
(Solution temperature and solution density with void evaluation)

Solution temperature convergence



Density convergence



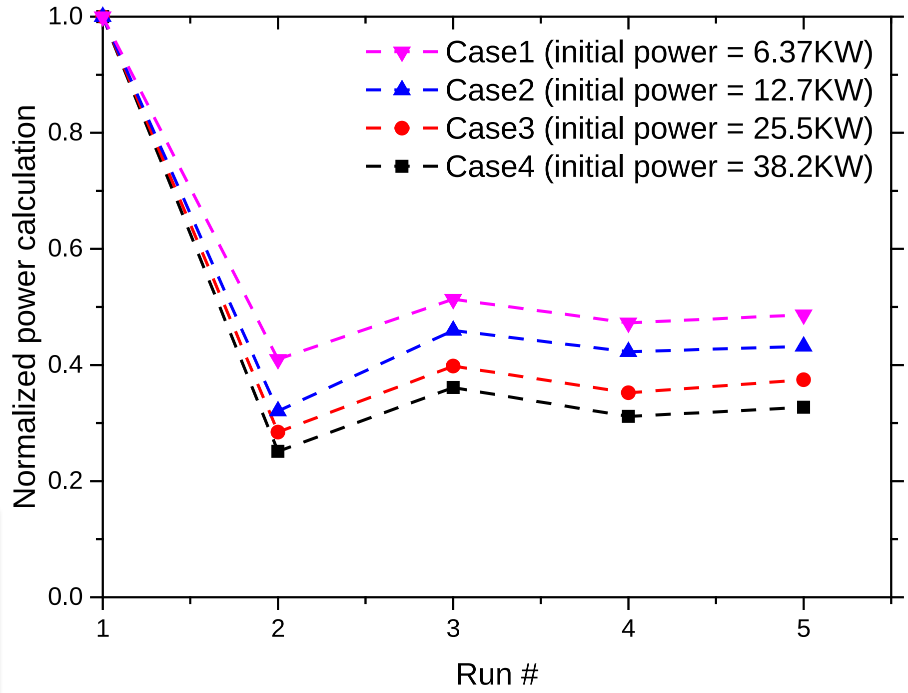


Accurate void profile calculation in MCFD results in realistic density and power calculation in fissile solution vessel

CASE study with different source neutron conditions

Test matrix for CASE study

	SN	Power converging (initial → saturated)
CASE1	1.458e14 [s^{-1}]	6.37 → 3.07KW (0.5KW/L → ~0.25 KW/L)
CASE2	2.916e14 [s^{-1}]	12.7 → 5.49KW (1.0KW/L → ~0.44 KW/L)
CASE3	5.832e14 [s^{-1}]	25.5 → 9.4KW (2.0KW/L → ~0.74 KW/L)
CASE4	8.745e14 [s^{-1}]	38.2 → 12.5KW (3.0KW/L → ~0.99 KW/L)



* Four source neutron cases are selected to target the initial power density ranging from 0.5 ~ 3 KW/L, resulting in saturated power density range from 0.25 ~ 1 KW/L.

* Gas generation rate is proportional to the power
: a constant conversion factor (1W ←→ 2.78e-9 kg/s) used

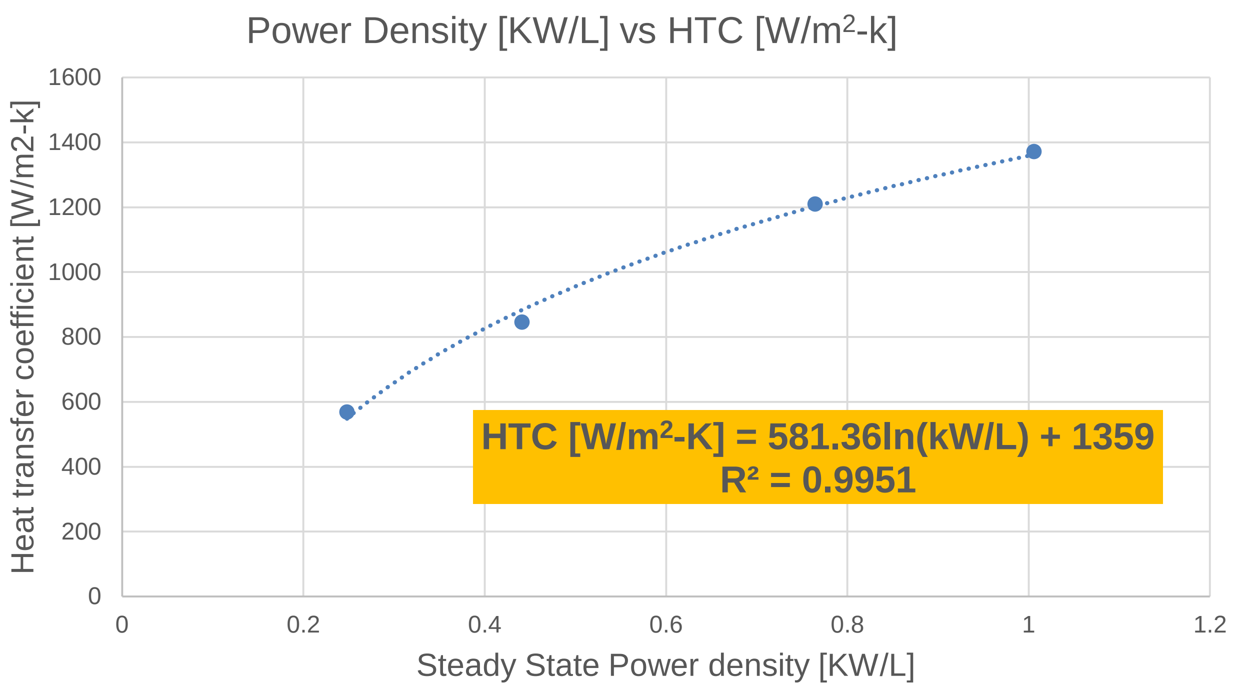
* Radiolytic gas bubble diameter is calculated based on simulations matching volume fraction measurements from L.D.P. King's paper on the SUPO reactor (1995) → D[mm] = 0.653 [Kw/L] + 0.11

Normalized saturated power (run#5) decreases as the power increases

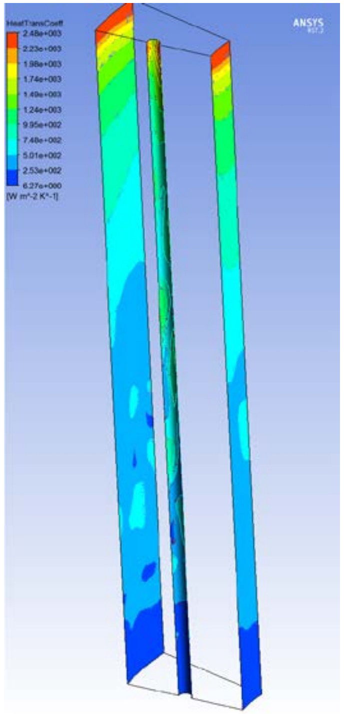
→ Case 1 : Saturated at 52% of initial power
→ Case 4 : Saturated at 32% of initial power

HTC correlation development for solution vessel

(correlation is based on the results of 4 case study)



HTC calculation from MCFD

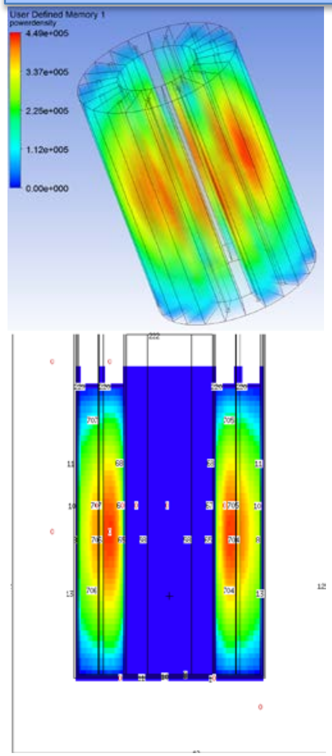


- A HTC correlation is developed in a range of 0.25KW/L ~ 1KW/L
- Overall HTC is evaluated via 1) lumped approach and 2) CFD post-analysis. Two method produce similar HTCs.
- HTCs from the current calculation can be used for the system code (e.g. SimApp) analysis in both steady state and transient mode.

Incremental methodology development

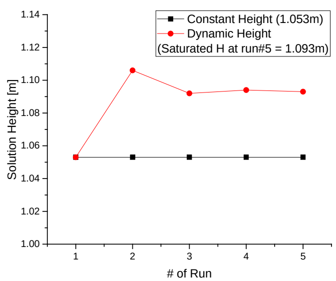
by implementing realistic system characteristics

Method-I
- Single-cell approach
- Constant Height



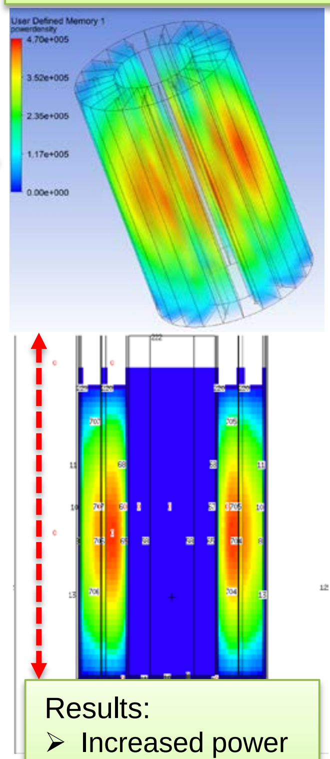
Fissile mass balance concept

$$V_1\rho_1 = V_2\rho_2$$
$$(mass\ conservation)$$
$$\therefore H_2 = H_1\frac{\rho_1}{\rho_2}$$



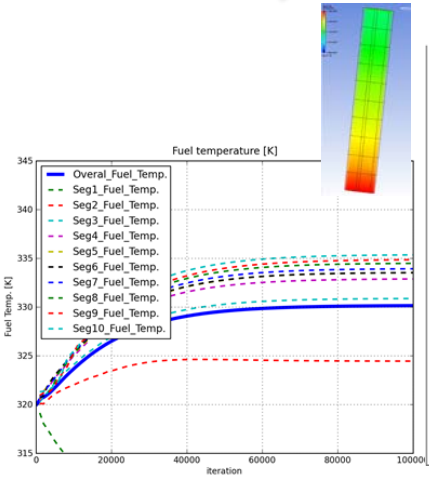
Solution height

Method-II
- Single-cell approach
- **Height adjustment**



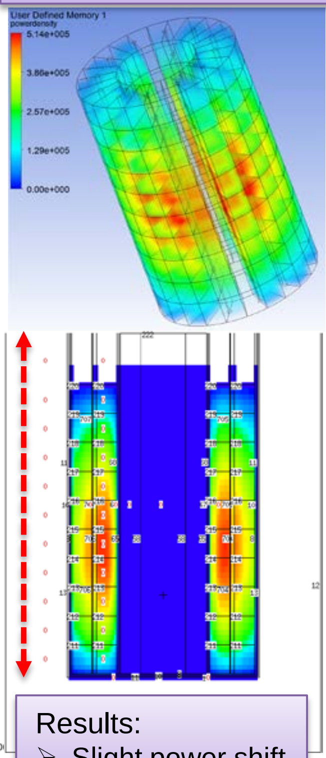
Results:
- Increased power
- Increased height

- Fissile mass balance
+
- **Heterogeneous density**



Solution temp.

Method-III
- **Multi-cell approach**
- **Height adjustment**

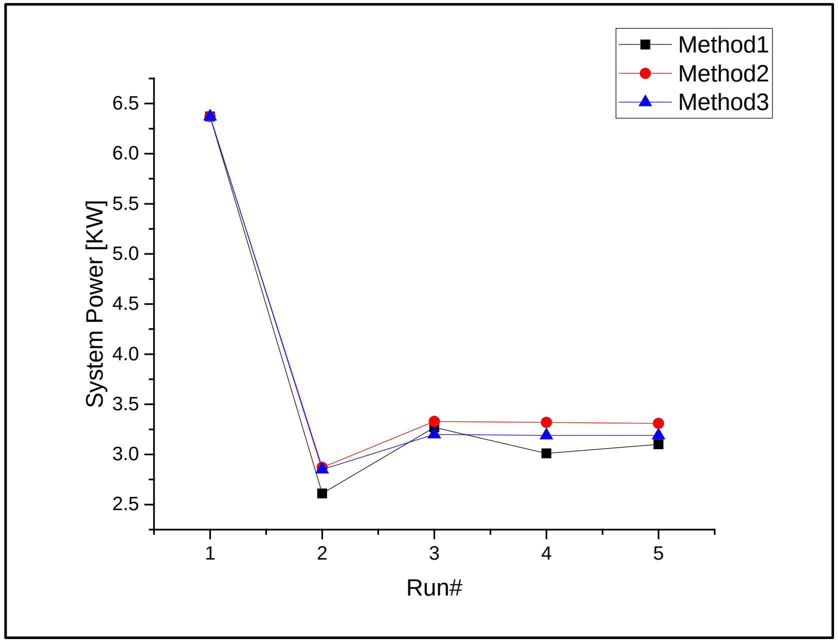


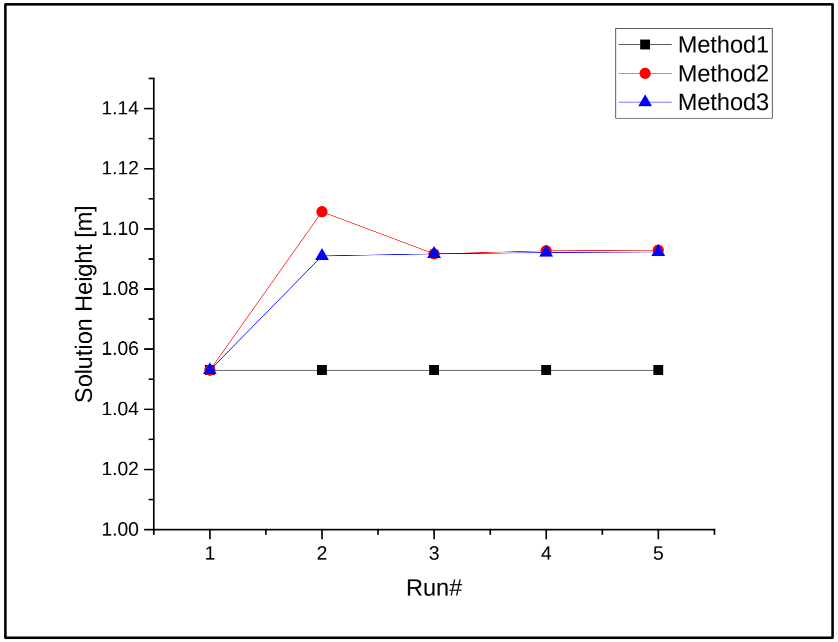
Results:
- Slight power shift

How calculation Methods affect system analysis

(CASE1, power and height)

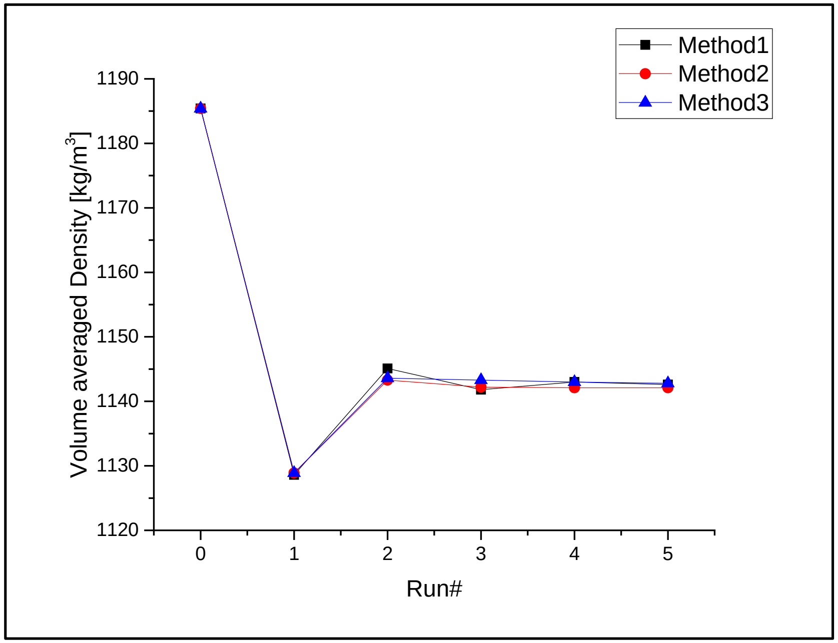
Power for 1/24th section

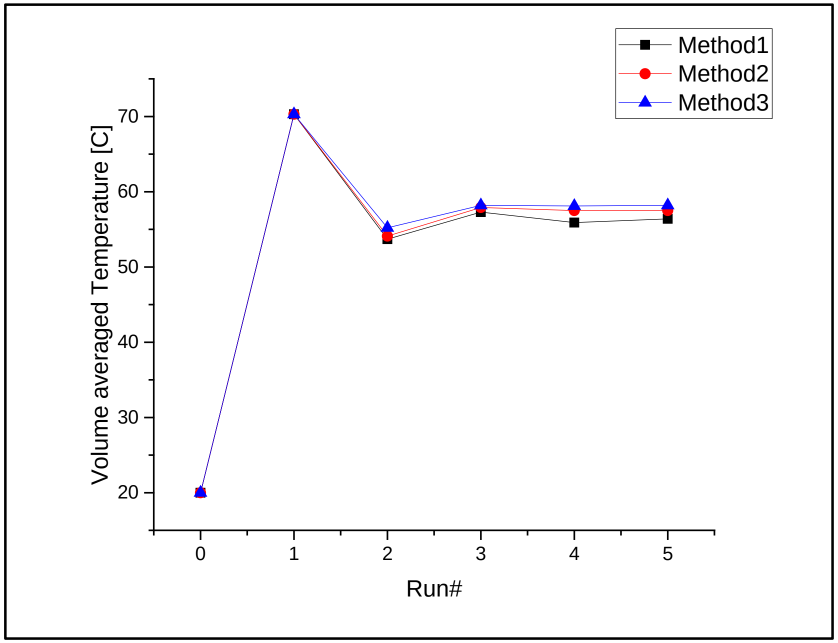




- **Improved Methods(2&3) predict higher system power compared to the original method**
- **Improved Methods (2&3) reach to a converged system condition quickly (mostly, after 3rd iteration)**
- **Solution height prediction by Method2 and Method3 are identical, with consideration of computational cost, Method2 would be the most practical coupled calculation approach for the current application.**

solution density and temperature for CASE1





Summary and path forward for Future works

Key findings from present study

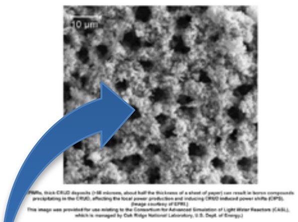
- A fully coupled neutronic and thermal hydraulic calculation method is demonstrated for Fissile solution vessel application in Mo99 technology
- Four different source neutron strength cases are selected to perform steady state power calculation and a corresponding HTC correlation is proposed.
- With the proposed system design, The achievable maximum power density would be 0.73KW/L with initial SN of 5.83e14 s^{-1}. *(Note that system may start boiling beyond the maximum power density)*
- Two improved calculation method (dynamic height adjustment & multi-cell approach) are proposed to establish a realistic model maturity. *(Note that Method2 would be reasonable coupled calculation approach for the current application)*

Potential future works

- Perform steady-state coupled calculations on various system configurations (i.e. varying aspect ratio and varying cooling tube #)
- Conduct a transient coupled calculation to evaluate transient system behavior

A thought developed from the current coupling analysis…

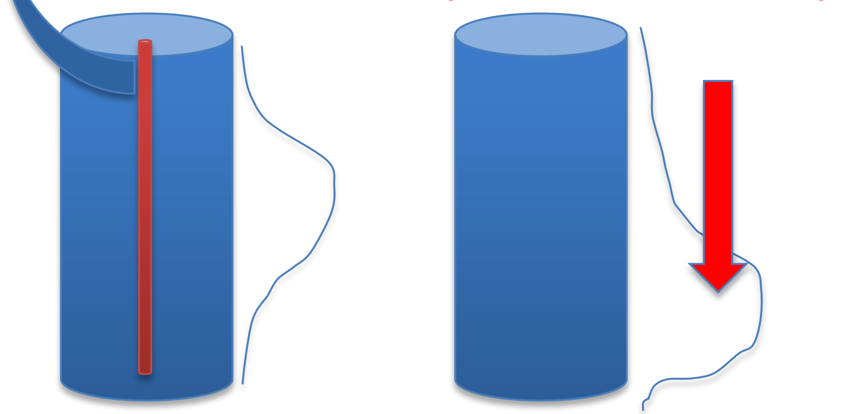
Power shift due to potential heterogeneous nature of Liquid Fueled Reactor (LFR)



CRUD induced power shift in LWR
Unexpected negative feedback from CRUD

Designed power profile
at normal condition

Actual power profile
(downward POWER shift)

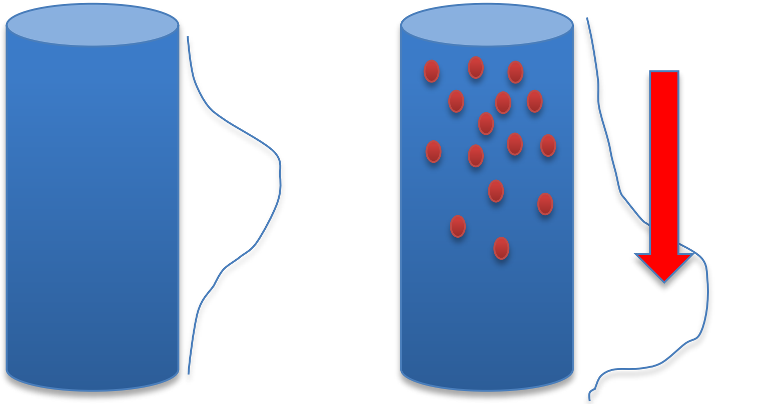


LWR application

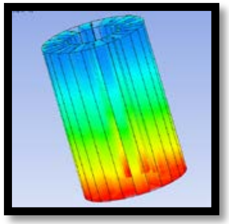
- Radiolytic gas bubble could lead negative reactivity at upper portion of solution
- Further investigation required to better understand the reactor kinetic in LFR design and TH safety issue.

Designed power profile
at normal condition

Actual power profile
(downward POWER shift)



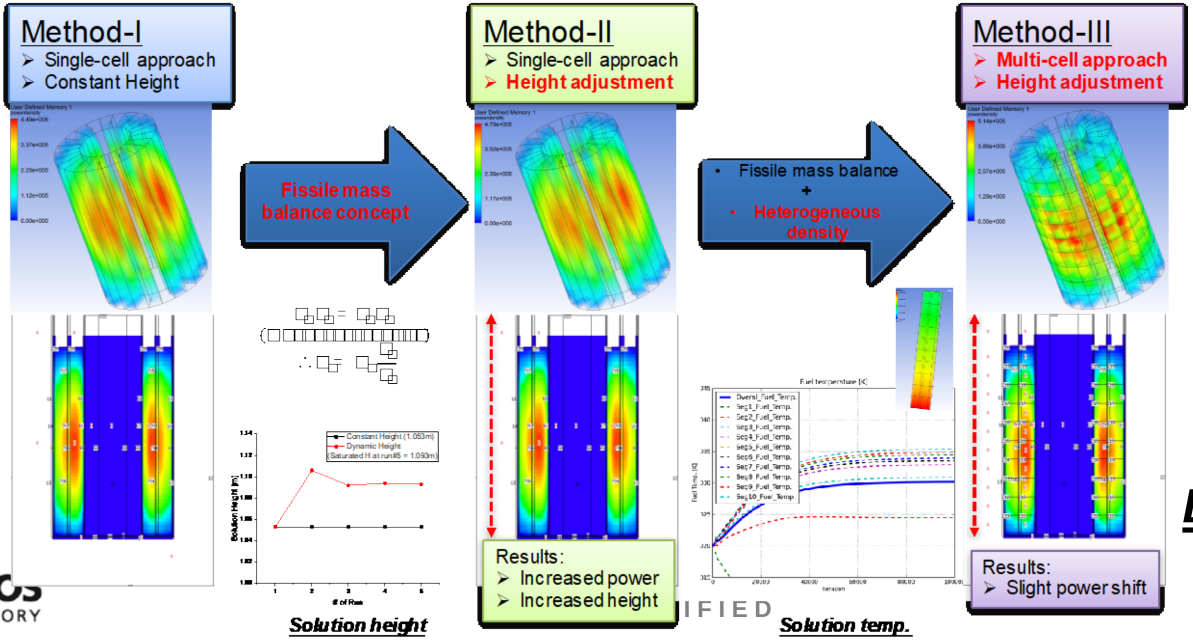
LFR application



Same Phenomena caused by different issue in LWR and LFR applications

Thanks for your attention
Q&A

Seung Jun Kim (skim@lanl.gov)



Backup slides…