Development and Qualification of State-of-the-Art Subchannel Methods for Advanced Reactors

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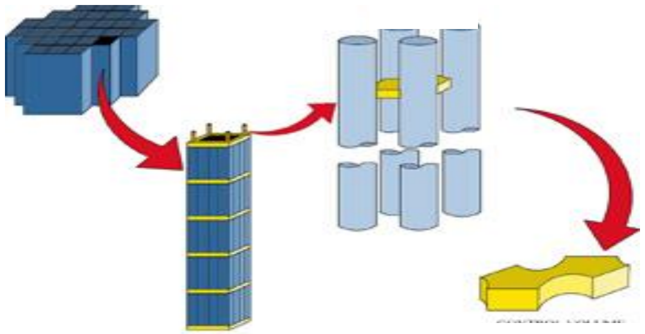
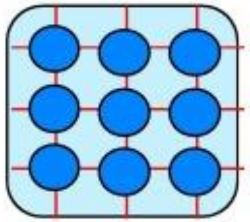
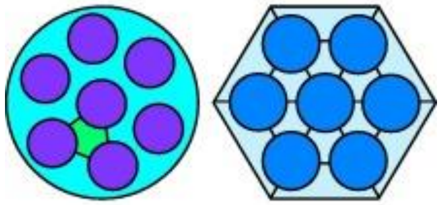
Subchannel Analysis Codes



Fuel Assembly



Square Pitch



Triangular Pitch

- In the subchannel analysis codes, the control volume is of a size equivalent to: (1) a single fuel rod and its associated fluid; or (2) a fluid volume bounded by four (three) fuel rods.
- Calculate detailed Thermal-Hydraulic (TH) conditions within subchannels (flow, enthalpy, pressure, void fraction, DNBR) and temperature distribution within fuel rod.
- Used to evaluate available / required thermal margins; number of failed rods due to DNB during accidents (*historically, developed and utilized mostly for LWR analysis*).

Subchannel Analysis Codes

- Traditionally, thermal-hydraulic sub-channel codes have been used:
  - either for standalone rod bundle TH Modeling and Simulation (M&S) on a sub-channel level,
  - or for coupled TH with neutronics reactor core M&S on a fuel assembly level.
- As part of integrated safety capability developments, thermal-hydraulic sub-channel models have been utilized for both hot fuel assembly and whole core analysis in one-way coupling using pin-power reconstruction techniques.
- Lately within large US national and international projects, TH sub-channel codes are being coupled with neutron transport codes and fuel performance codes for high-fidelity reactor core M&S on a pin (sub-pin)/sub-channel level.

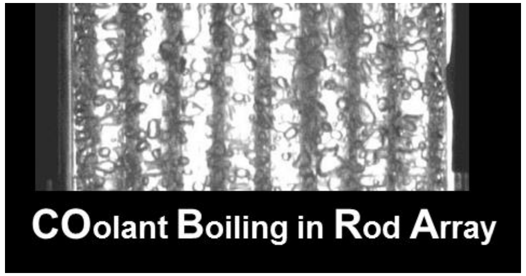
‼ To make these high-fidelity multi-physics codes accurate and efficient, developments are needed to improve the individual physics components as well as the coupling between them.

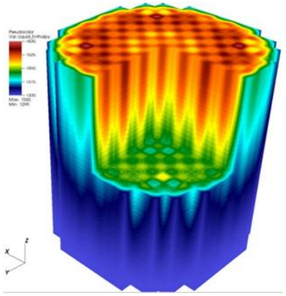
Subchannel Analysis Codes for Advanced Reactors

- Although recently there have been promising developments (mostly in China and Japan) in applying subchannel analysis to liquid metal cooled fast reactors, substantial developments (supplemented with Verification, Validation and Uncertainty Quantification (VVUQ) are yet needed:
  - new physics to account for (underlying assumptions; EoS & closures)
  - material properties (coolant, fuel, structures);
  - geometry and changes in geometry (feedback to neutronics);
  - numerical stability; etc.
- *Let us use as an example the subchannel code CTF.*

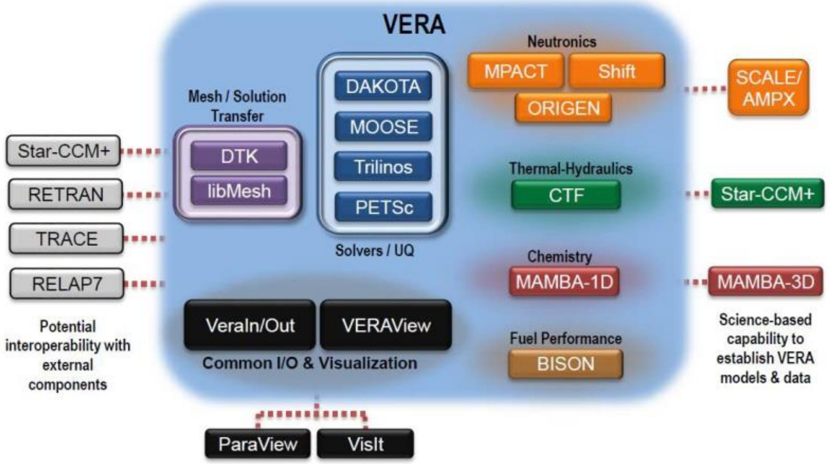
Subchannel Analysis Code CTF

CTF originates from COBRA-TF family codes - two-fluid three-field two-phase flow model in subchannel resolution





CTF is jointly developed by RDFMG-NCSU and ORNL within DOE CASL project



The well-established users' group (CTF UG) holds annual meetings to discuss code developments, improvements, multi-physics and multi-scale coupling, verification, validation, uncertainty quantifications, and applications.

CTF provides the best available sub-channel methods for LWR analysis.

Developments (primarily at ORNL) for enabling CTF for solid fuel molten salt reactor modeling are ongoing.

Ongoing work at NC State to extend the CTF modeling capabilities to Sodium Fast Reactors (SFRs).

Enabling CTF for SFRs: CTF-R

- CTF is a state-of-the-art thermal-hydraulics subchannel code designed for LWRs vessel and core analysis.
- The code solves a coupled system of mass, momentum, and energy conservation equations for liquid, vapor, and liquid drop flow fields.
- CTF has been extensively developed and validated for water cooled reactors ONLY!
- Initial attends to apply CTF to SFRs were unsuccessful because of the code underlying assumptions; closures; and numerical solution scheme.
- Enabling CTF for SFRs (and other fast liquid metal cooled reactors) is one of the driving forces behind the CTF-Residual (CTF-R) development.

CTF-Residual (CTF-R): Theory Review

Conservation Equations:

- Current implementation of CTF-R is single phase with friction, lateral transfer, and simplified fuel rod model.
- Five conservation equations: mass, axial momentum, lateral momentum, and energy of the fluid, as well as energy of the solid:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho w}{\partial z} - \kappa_1 \frac{\partial^2 \rho}{\partial z^2} = 0$$

$$\rho \frac{\partial h}{\partial t} + \rho u \frac{\partial h}{\partial x} - \frac{\partial P}{\partial t} + \frac{\partial \rho h w}{\partial z} - \kappa_2 \frac{\partial^2 h}{\partial z^2} = \frac{S_{ht}}{V}$$

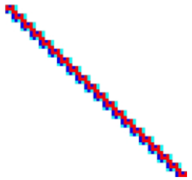
$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial P}{\partial x} + \frac{1}{\rho}\frac{\partial \rho u w}{\partial z} - \frac{\kappa_3}{\rho}\frac{\partial^2 u}{\partial z^2} = g + S_f$$

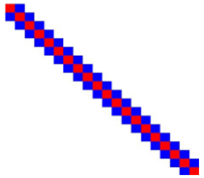
$$\frac{\partial w}{\partial t} + \frac{1}{\rho}\frac{\partial P}{\partial z} = H|w|w$$

$$M c_p \frac{\partial T}{\partial t} = \sum_x q_s'' A_s + q''' V - S_{ht}$$

CTF-Residual (CTF-R): Theory Review

Jacobian Construction:





- The pressure matrix in CTF is coded analytically.

- CTF-R constructs the Jacobian by numerically perturbing the conservation equations.

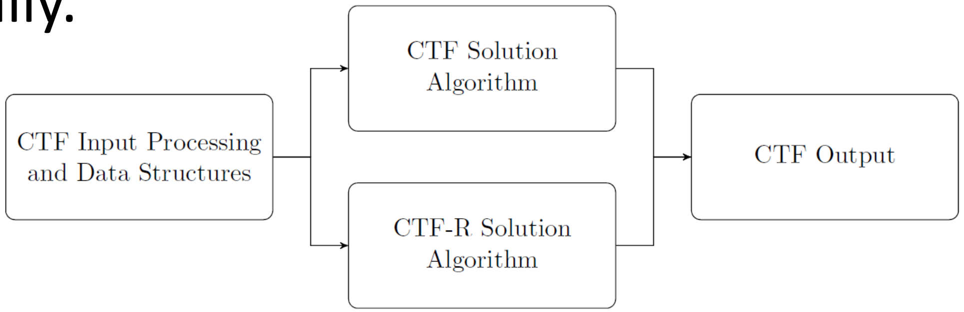
$$J\delta x = F(x)$$

$$J = \frac{\partial F_j(x)}{\partial x_i} = \frac{F_j(x_i + \epsilon) - F_j(x_i)}{\epsilon}$$

- Where F is a conservation equation and x is the array of solution variables.

- The discrete equations are linearized, so this is exact.

CTF-Residual (CTF-R): Motivation



- Keep CTF input/output, build the Jacobian numerically.
- Flexibility:
  - Add/remove or change conservation equations;
  - Can change the implicitness of the Jacobian;
  - Construction of the pressure or Jacobian matrix in a variety of ways;
  - Direct steady state solution.
- Readability:
  - Ease of use and reduces development time;
  - Naturally couples to PETSc or other numerical solvers;
  - Tight coupling to other codes through sharing a Jacobian matrix is a possibility.
- CTF-R can be easily adapted to different reactor types, while CTF is mostly restricted to LWR simulations.

SFR TH Modeling with CTF-R

- Our Goal: To enable CTF-R for SFR thermal-hydraulics modeling and simulation.
- Need to explore the underlying assumptions:
  - *What assumptions do we make in the current CTF-R solution? If these are applicable to sodium? If not, how do we change them?*
  - *An example: the thermal and viscous boundary layers are approximately equal in water; however, the thermal boundary layer is much thicker in sodium. This greatly changes the formulation of the governing equations and closures.*
- Required improvements & developments:
  - *Coolant (sodium) properties;*
  - *Coolant mixing;*
  - *Friction pressure losses;*
  - *Heat conduction in sodium;*
  - *Verification & Unit Testing;*
  - *Validation & UQ.*

SFR TH in CTF-R: Sodium Properties

- Correlations are compiled from various sources.
- Ranges of validity for liquid sodium are:
  - *Temperature (97.8 ^{o}C to 873.0 ^{o}C) & Pressure (10 Pa to 10^{7} Pa)*
- Typically, SFR operates with a primary sodium temperatures between 360 ^{o}C and up to 545 ^{o}C.
- CTF-R models heat transfer to the coolant by calculating convective heat transfer coefficients from the Nusselt number:
  - *A correlation for Nusselt number developed by Borishanskii et al. is used for sodium coolant.*
  - *The correlation is valid for pitch-to-diameter ratio between 1.1 and 1.5, and Péclet number up to 2000.*

$$Nu = 24.15\, log\left[-8.12 + 12.76\left(\frac{P}{D}\right) - 3.65\left(\frac{P}{D}\right)^2\right] + 0.0174\left[1 - exp\left(6 - 6\left(\frac{P}{D}\right)\right)\right][Pe - 200]^{0.9} \quad 200 < Pé \leq 2000$$

$$Nu = 24.15\log\left[-8.12 + 12.76\left(\frac{P}{D}\right) - 3.65\left(\frac{P}{D}\right)^2\right] \quad Pé \leq 200$$

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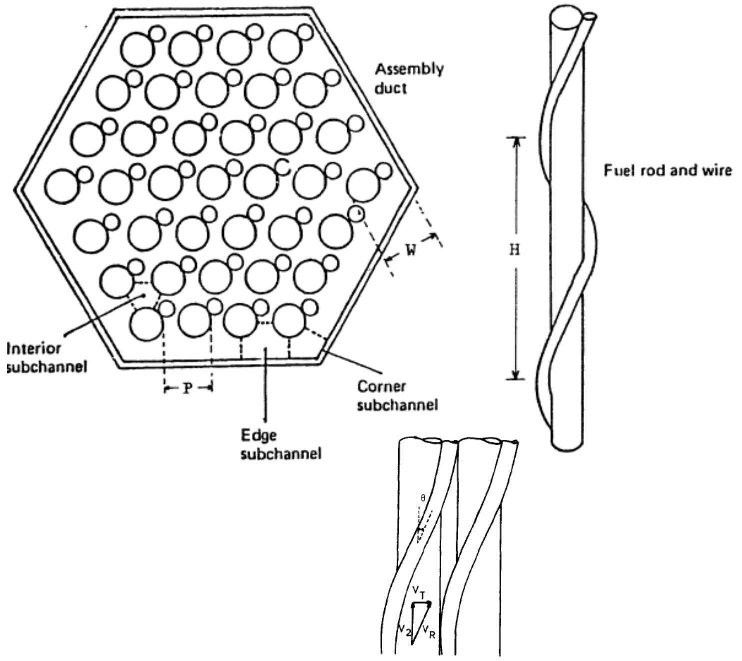
SFR TH in CTF-R: Coolant Mixing

- Wire-wrapping is used for continuous structural support in contrast to the localized spacer grids used in LWRs.
- This generates a forced lateral flow due to the wire drag that contributes to the flow mixing.
- The effective mixing flow rate W_{ij} is defined as: $W_{ij} = \beta_i s_{ij} \overline{G_k}$.
- The mixing coefficient β_i is determined from empirical correlations.
- The approach differentiates between the interior channels and edge channels mixing:
  - *Interior region: mixing is due to the lateral enhanced eddy diffusivity (ϵ^*).*
  - *Edge region: uniform transverse velocity V_T (C_{1L}).*
  - *Both parameters are integral values over the wire lead length (H).*
- Cheng & Todreas correlation:
  - *Interior region: (Eddy diffusivity):* $\epsilon^* = C_m \left(\frac{A_{r1}}{A_1'}\right)^{1/2} \tan(\theta)$.
  - *Edge region: (uniform transverse velocity):* $C_{1L} = C_s \left(\frac{A_{r2}}{A_2'}\right)^{1/2} \tan(\theta)$.



Bare rod flow area and wetted perimeter

$A_1' = (\sqrt{3}/4)P^2 - \pi D^2/8$,

$A_2' = P\left(W - \frac{D}{2}\right) - \pi D^2/8$,

$A_3' = \left((W - D/2)^2/\sqrt{3}\right) - \pi D^2/24$,

$A_b' = N_1 A_1' + N_2 A_2' + N_3 A_3'$,

$P_{w1}' = \pi D/2$,

$P_{w2}' = P + \pi D/2$,

$P_{w3}' = \pi D/6 + 2(W - D/2)/\sqrt{3}$,

$P_{wb}' = N_1 P_{w1}' + N_2 P_{w2}' + N_3 P_{w3}'$.

Wire-wrapped flow area and wetted perimeter

$A_1 = A_1' - \pi D_w^2/(8\cos\theta)$,

$A_2 = A_2' - \pi D_w^2/(8\cos\theta)$,

$A_3 = A_3' - \pi D_w^2/(24\cos\theta)$,

$A_b = N_1 A_1 + N_2 A_2 + N_3 A_3$,

$P_{w1} = P_{w1}' + \pi D_w/(2\cos\theta)$,

$P_{w2} = P_{w2}' + \pi D_w/(2\cos\theta)$,

$P_{w3} = P_{w3}' + \pi D_w/(6\cos\theta)$,

$P_{wb} = N_1 P_{w1} + N_2 P_{w2} + N_3 P_{w3}$,

where $\cos\theta = H/\sqrt{H^2 + (\pi(D + D_w))^2}$.

Wire projected area

$A_{r1} = \pi(D + D_w)D_w/6$,

$A_{r2} = \pi(D + D_w)D_w/4$,

$A_{r3} = \pi(D + D_w)D_w/6$.

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SFR TH in CTF-R: Friction Pressure Losses

- The axial flow resistance R_z is expressed in terms of the pressure drop equation:

$$R_z = f_z \frac{\rho w^2}{2D_h}$$

- f_z (axial pressure drop coefficient) is determined empirically.
- The simplified Cheng & Todreas friction factor correlation is used in CTF-R to model pressure drop.

The simplified Cheng and Todreas (1986) correlation

For laminar region, $Re < Re_L$

$$f = C_{fL}/Re \quad \text{(B6)}$$

For turbulent region, $Re > Re_T$

$$f = C_{fT}/Re^{0.18} \quad \text{(B6.1)}$$

For transition region, $Re_L \leqq Re \leqq Re_T$

$$f = (C_{fL}/Re)(1-\Psi)^{1/3} + (C_{fT}/Re^{0.18})\Psi^{1/3} \quad \text{(B6.2)}$$

where

$$Re_L = 300(10^{1.7(P/D-1.0)}) \quad \text{(B6.3)}$$

$$Re_T = 10,000(10^{0.7(P/D-1.0)}) \quad \text{(B6.4)}$$

$$\Psi = \log(Re/Re_L)/\log(Re_T/Re_L) \quad \text{(B6.5)}$$

$$C_{fL} = (-974.6 + 1612.0(P/D) - 598.5(P/D)^2)(H/D)^{0.06-0.085(P/D)} \quad \text{(B6.6)}$$

$$C_{fT} = (0.8063 - 0.9022(\log(H/D)) + 0.3526(\log(H/D))^2) \times (P/D)^{9.7}(H/D)^{1.78-2.0(P/D)} \quad \text{(B6.7)}$$

SFR TH in CTF-R: Heat Conduction in Sodium

- Because sodium has a much higher thermal conductivity than water, the conduction inside the fluid is more influential (this is especially true for natural circulation conditions).
- In CTF, the heat conduction in the coolant is neglected due to the lower thermal conductivity of water.
- In CTF-R, the heat conduction term is re-inserted into energy equation when sodium coolant is modeled:
  - *The heat conduction term is derived and coded in the subchannel energy equation form;*
  - *The temperature gradient is taken across the gap's mixing length;*
  - *The heat conduction term is on the form:* $q'' = K\left(\frac{dT}{dX}\right)_{gap}$;
  - *The mean thermal conductivity is obtained by averaging the thermal conductivity between two adjacent subchannels connected by a gap:* $q'' = \eta K\left(\frac{Ti-Tj}{l_{ij}}\right)_{gap}$;
  - *The conduction shape factor is geometry-dependent. It is approximated in CTF-R using the correlation by Jeong et al. :* $\eta = 0.777\left(\frac{P}{D}\right)\left(\frac{S}{D}\right)^{-0.263}$.

SFR TH in CTF-R: Thermal Expansion

- Motivation: To replicate the effect of thermal expansion on the fuel material density for reactivity feedback modeling in multi-physics simulations of liquid metal fast breeder reactors by estimating the new materials number densities and thus neutron macroscopic cross sections.
- Challenges: To model thermal expansion, we need a discretization method that would change the size of each node for each time step (either through change in node size or through moving cell boundaries).
- Solution: The current objective is to replicate the effect of thermal expansion without changing the existing mesh dimensions in CTF-R:
  - *To achieve it, no re-meshing is required: new density at every axial location is calculated using thermal expansion coefficient based on the current temperature at every axial node calculated by CTF;*
  - *Set of metallic fuels and alloys and their corresponding thermal-expansion correlations is available in CTF-R.*

SFR TH in CTF-R: Test Cases and Validation

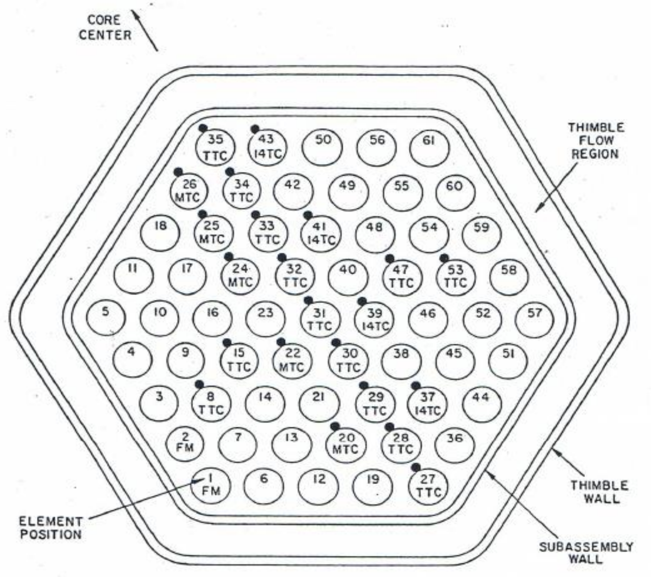
- CTF-R has been tested to verify its functionality for modeling SFR.
- CTF-R needs extensive validation work for SFR modeling and simulation.
- The first set of validation cases is based on the ANL/IAEA Benchmark steady state data for EBR-II Shutdown Heat Removal Tests (SHRT-17) and (SHRT-45R):

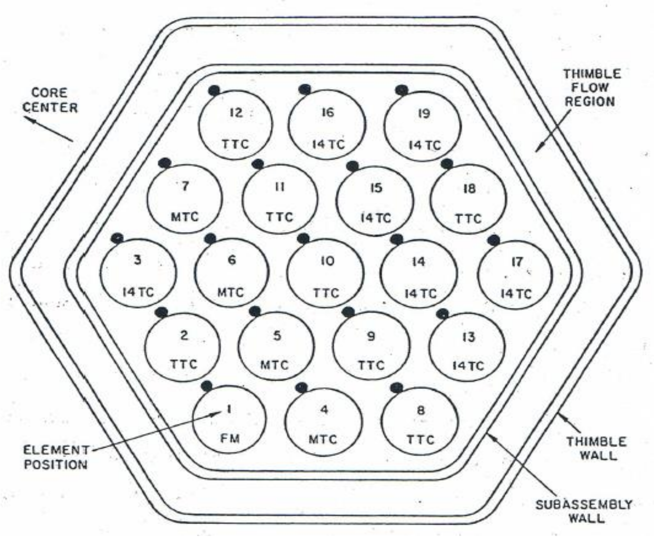
SHRT-17 was a loss of flow test. In this test, the reactor was operated at steady state power level of 57.3 MW until equilibrium condition were reached. The primary sodium flow rate was 0.54 kg/s calibrated at 426^{o}C. The transient was initialed by tripping the primary and intermediate sodium pumps. No auxiliary pumps were turned on which imitated the situation of a station blackout. The sodium flow coast down meant that the reactor was cooled by natural circulation. No action were taken by the operators until the experiment was over and the reactor conditions remained within safe limits.

SHRT-45 was a loss of flow test without protection. The control rods drivers were deactivated to prohibit control rods insertion or withdrawal by drive motors. The reactor was operated at steady state power of 60.0 MW and a primary sodium flow rate of 0.57 kg/s. Similar to the SHRT-17, the transient was initiated by tripping the primary and intermediate pumps. This time the control rods did not intervene. As the transient progressed, the reactor power decreased due to negative reactivity feedbacks and the reactor conditions were within safe limits during the whole run time of the transient.

SFR TH in CTF-R: Test Cases and Validation

- Subassemblies named XX09 (left) and XX10 (right) were equipped with mass flow meters and thermocouples at various radial and axial location in the core for cladding temperature measurements and the coolant inlet temperatures.

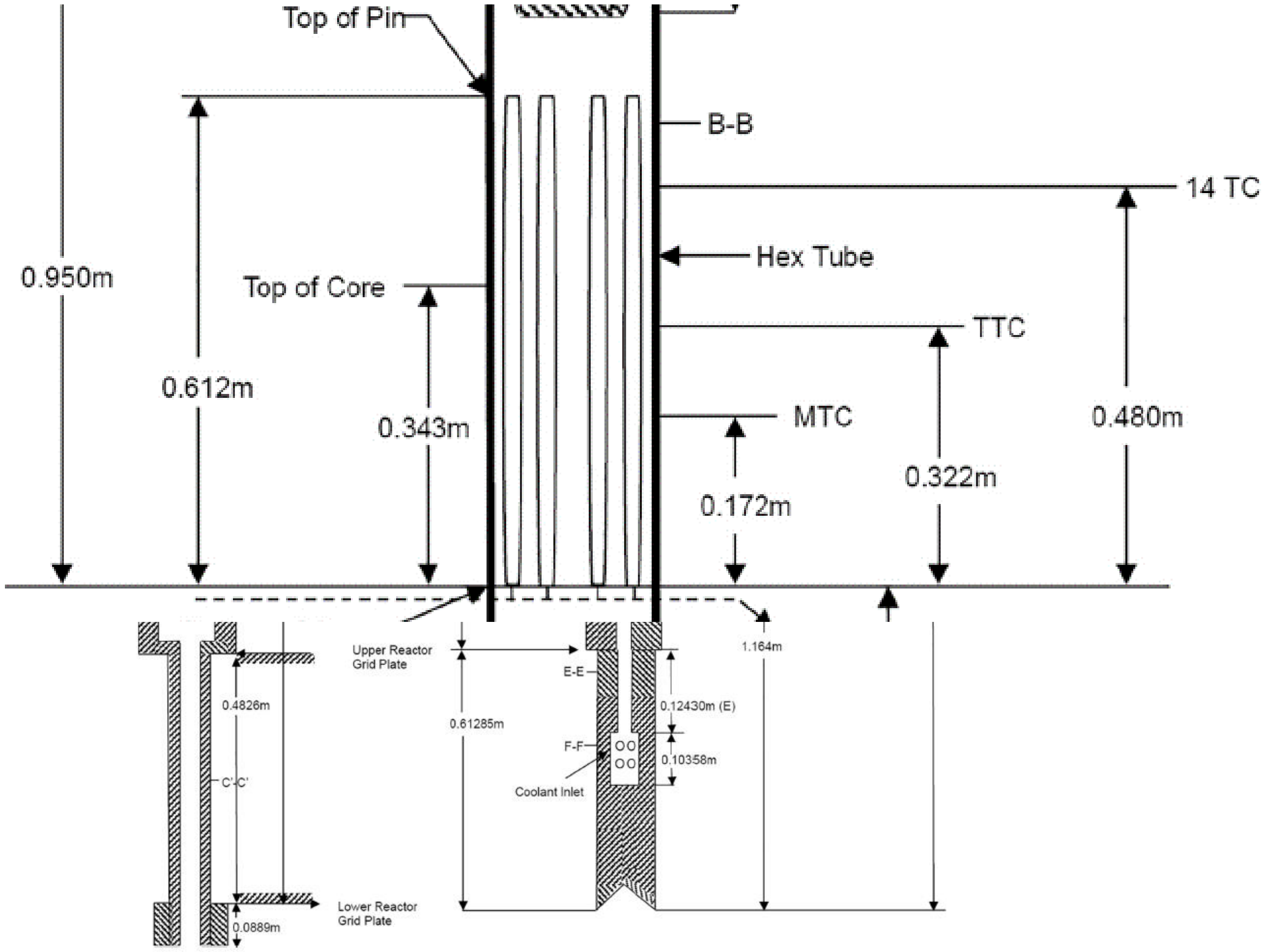




	XX09	XX10
Fuel alloy (wt %)	U-5Fs	Stainless Steel
Enrichment (wt% U235)	67	N/A
Number of elements	59/61	18/19
Fuel-slug length (m)	0.3429	N/A
Fuel-slug diameter (mm)	3.36	N/A
Cladding outer diameter (mm)	4.41	8.81
Pin pitch (mm)	5.664	10.058
Element length (m)	0.6108	0.6108
Cladding material	SS316	SS316
Spacer-wire diameter (mm)	1.24	1.24
Spacer-wire material	SS316	SS316
Inner Hex flat-to-flat inside (mm)	46.4	46.4
Inner Hex flat-to-flat outside (mm)	48.4	48.4
Outer hex flat-to-flat inside (mm)	56.1	56.1
Outer hex flat-to-flat outside (mm)	58.17	58.17
MTC axial location (m)	0.172	0.172
TTC axial location (m)	0.322	0.322
14TC axial location (m)	0.48	0.48

SFR TH in CTF-R: Test Cases and Validation

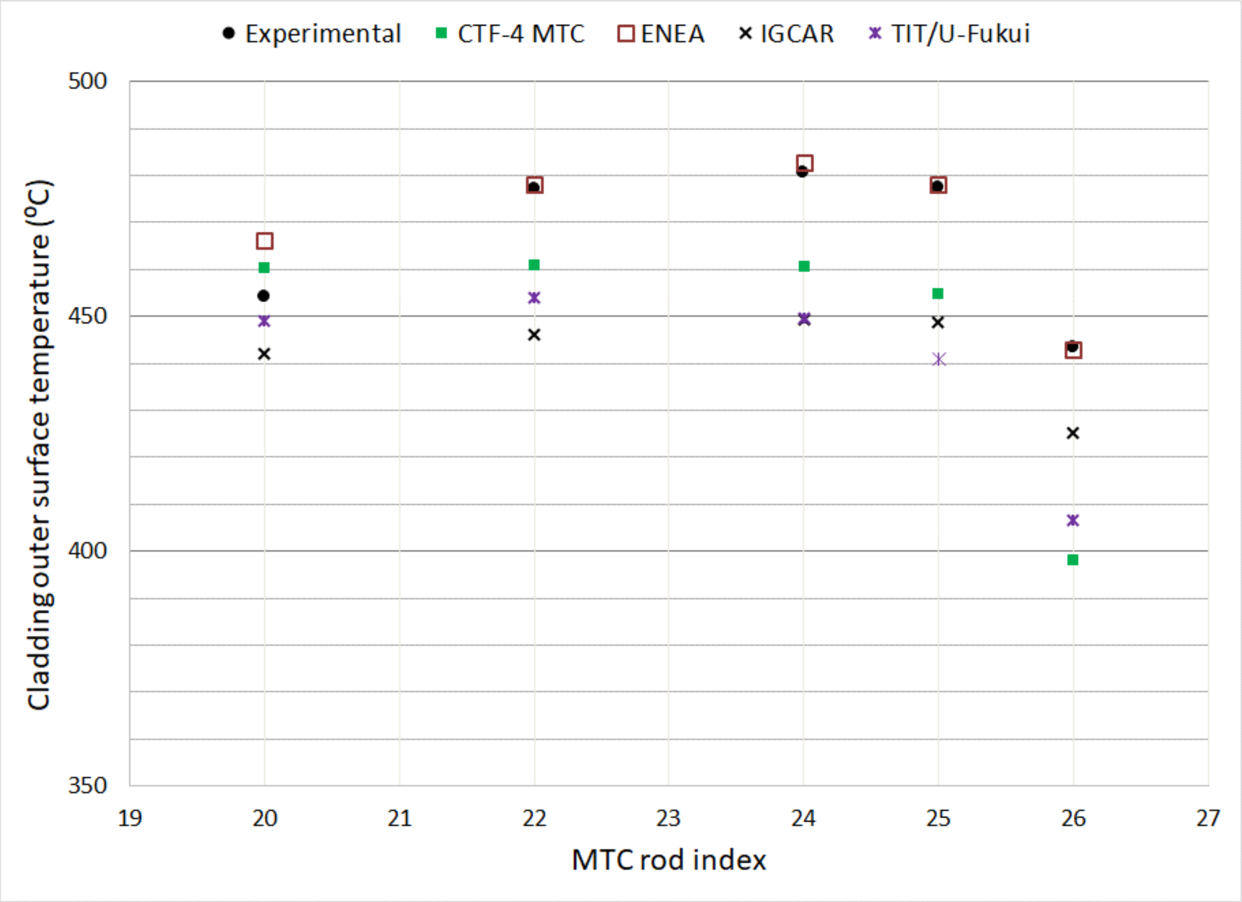
Schematics of instrumented subassembly XX09

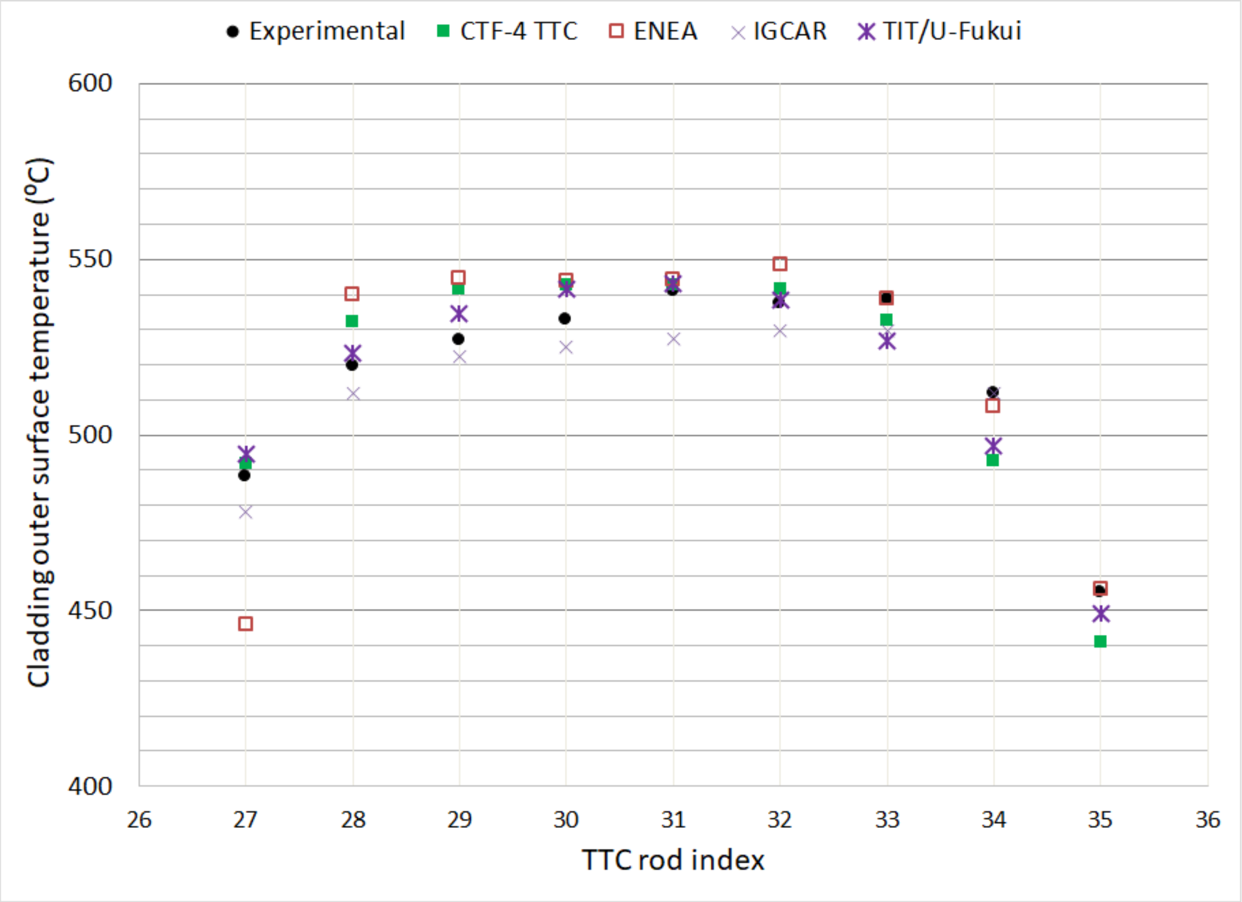


- The following figures illustrate results for XX09 and XX10 subassemblies at MTC (midplane thermocouple) and TTC (top-of-core thermocouple).
- The results were compared to the data in open literature (ANL/IAEA benchmark results).
- Data is extracted using WebPlotDigitzer app, which might create slight errors but without affecting the overall comparisons.
- ENEA and IGCAR used CFD methods, while TIT/U-Fukui used a version of the subchannel code COBRA-IV.

SFR TH in CTF-R: Test Cases and Validation

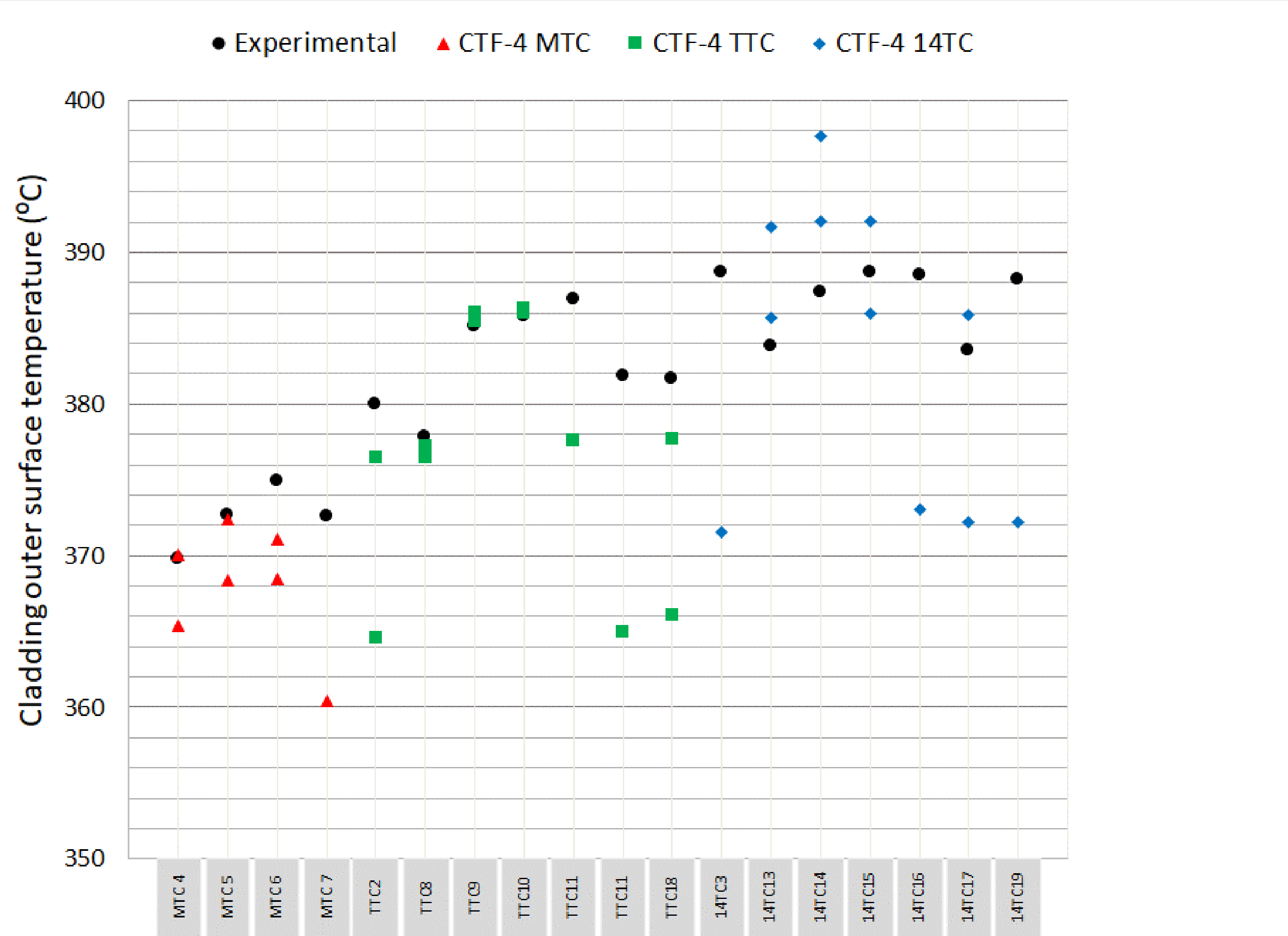
SHRT-17 XX09 Results:





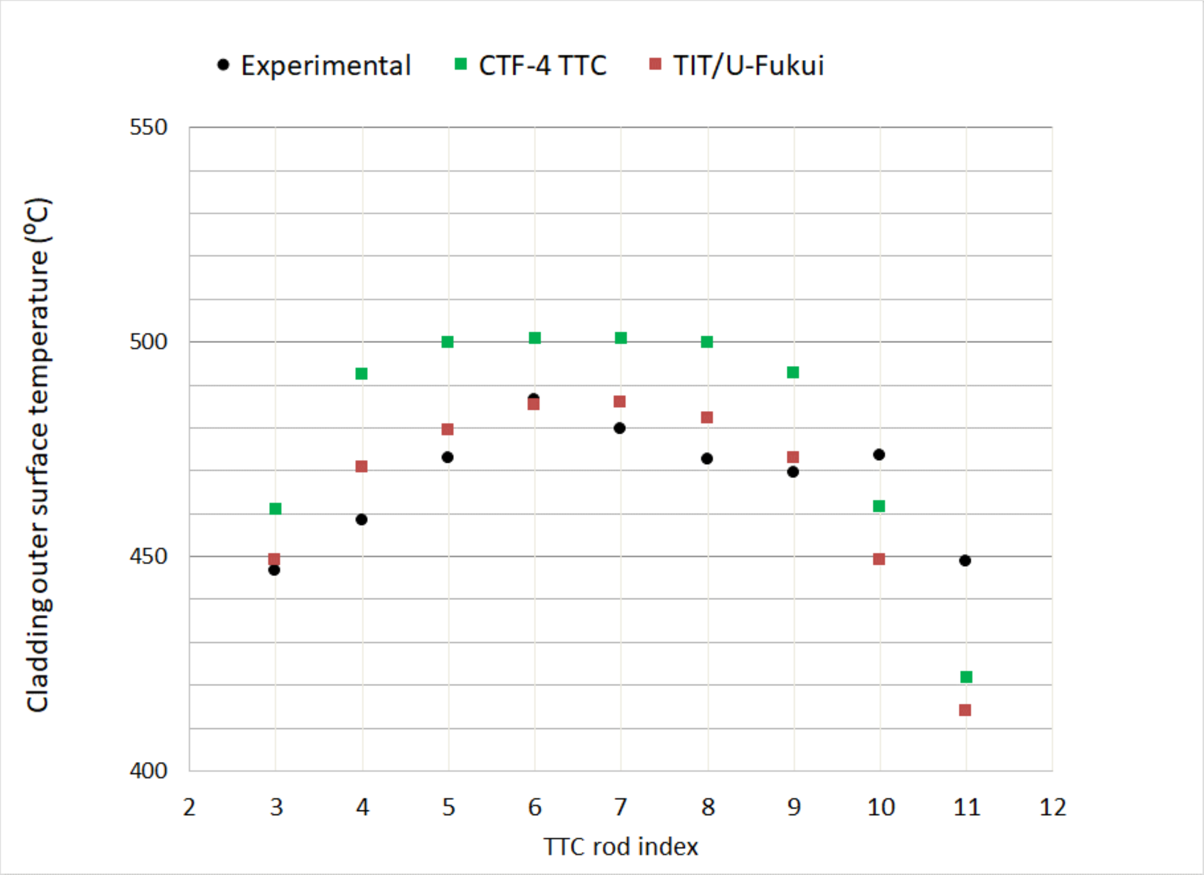
SFR TH in CTF-R: Test Cases and Validation

SHRT-17 XX10 Results:

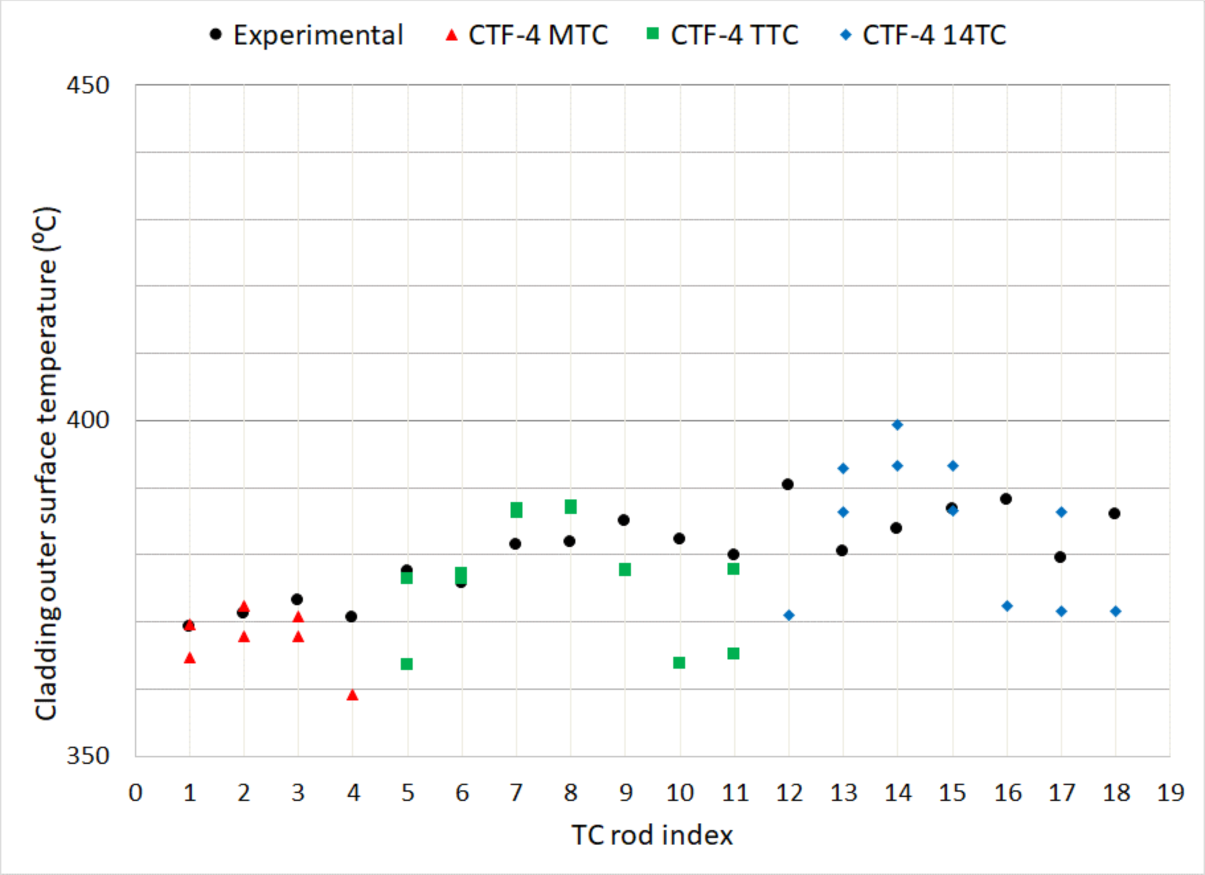


SFR TH in CTF-R: Test Cases and Validation

SHRT-45 XX09 Results:



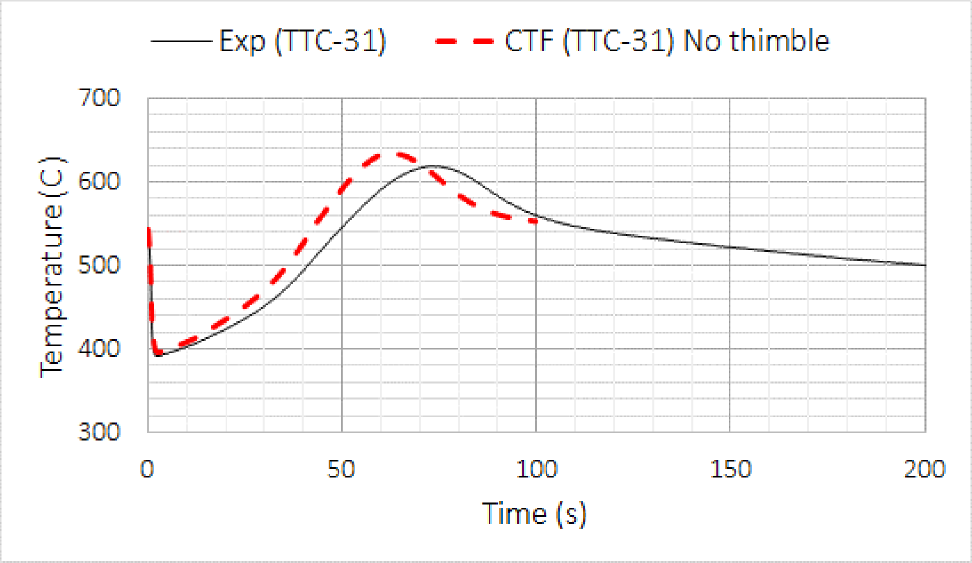
SHRT-45 XX10 Results:

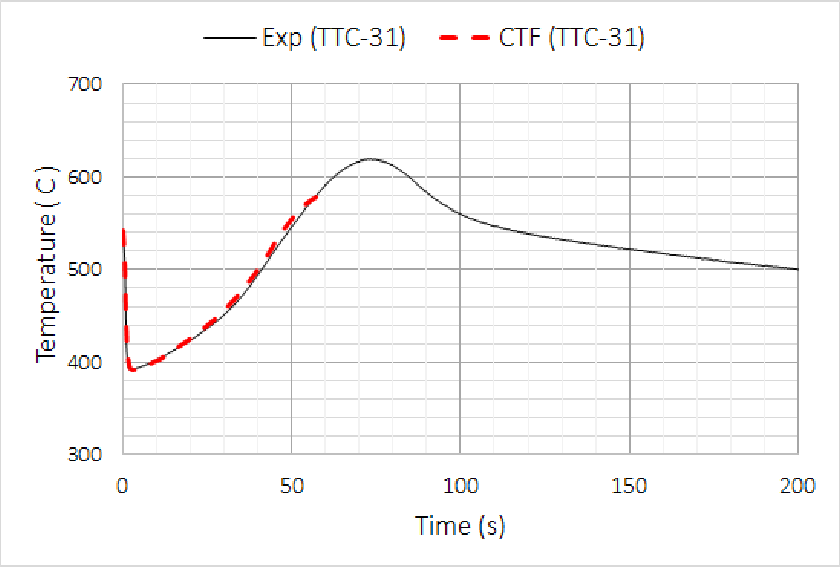


SFR TH in CTF-R: Test Cases and Validation

In Summary:

- The code predictions agreed with experimental results for XX10 in the two tests.
- Good agreement was also obtained for XX09 in SHRT-17 and a slight over-prediction in SHRT-45.
- The future work consists of modeling XX09 and XX10 subassemblies during the whole transient periods of SHRT-17 and SHRT-45.

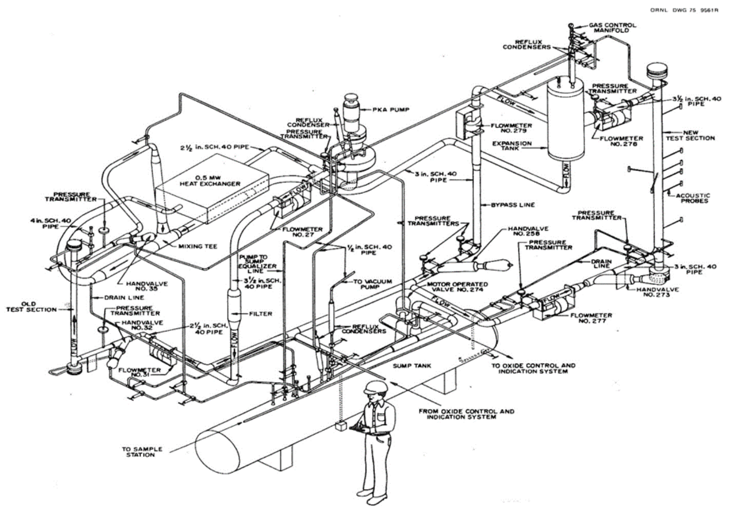


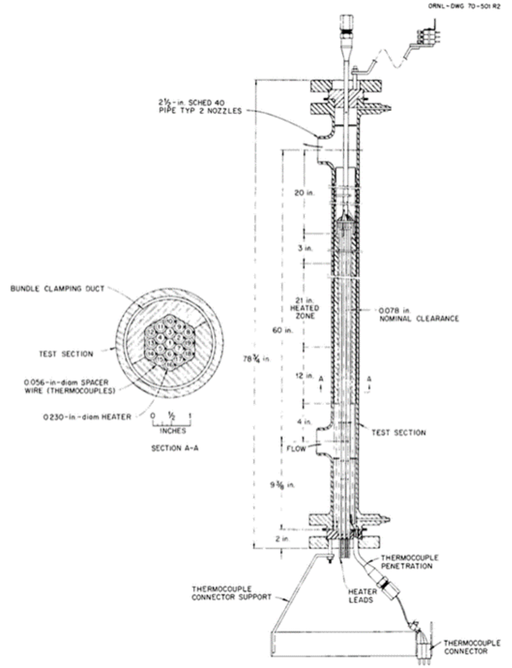


SFR TH in CTF-R: Test Cases and Validation

THORS Experimental Data and Benchmark:

- ORNL and NCSU are developing the benchmark specification for SFR Thermal-Hydraulic (TH) UAM benchmark exercise as part of the OECD/NEA SFR-UAM benchmark based on the Thermal Hydraulics Out of Reactor Safety (THORS) experimental loops data with an emphasis on high to low resolution model data exchange (Hi2Lo)
- THORS was a large high temperature sodium facility in which a number of bundles simulating SFR cores were tested.
- The measurements consist mostly of transient temperature fields in the wires and on the pin surfaces.
- Measurements of different pin/wires temperatures at several axial locations allow for reconstruction of the 3-D temperature flow field.
- Pressure drop measurements over the entire test section, flow rates, and acoustic signals for boiling detection were also conducted.

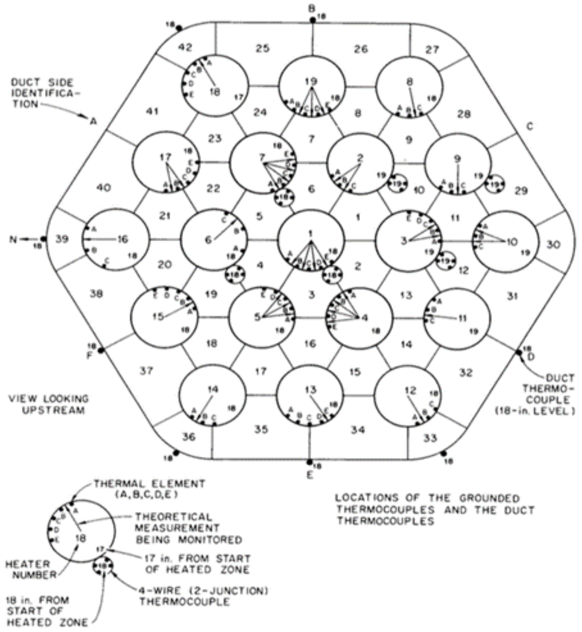


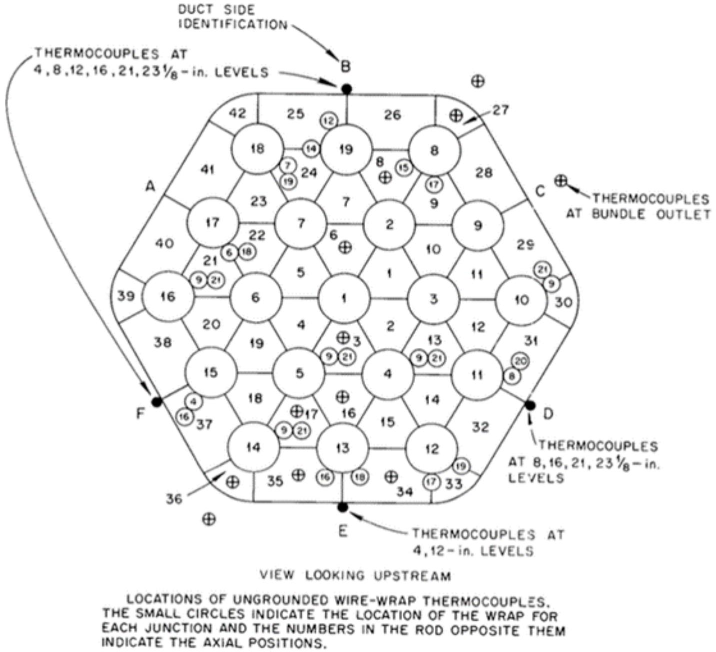


SFR TH in CTF-R: Test Cases and Validation

THORS Experimental Data and Benchmark:

- The objective of this TH benchmark exercise are:
  - To provide a sodium turbulent flow and heat transfer database for high resolution (CFD and Subchannel) model validation.
  - To emphasize the importance of uncertainty analysis for TH simulations for a variety of reasons.
  - To establish best practices for Quantification of geometry modelling, input data, fluid properties, and other uncertainties associated with the complex flows in wire wrapped pin arrays of SFR.
  - To develop guidance for CFD model/code validation for SFR fuel bundles that can be used to improve the existing standards.
  - To update the current generation TH models for pressure drop and inter-channel mixing and develop the hybrid experiment/simulation database necessary to establish and calibrate the low order models with high resolution (both experimental/numerical) data, e.g. Hi2Lo Problem.





SFR TH in CTF-R: Challenges in Validation

EoS & closures:

- Validation is important when implementing the new models;
- Lack of open (non-proprietary) validation data.

Effect of impurities on sodium properties:

- Implement a capability to estimate the effect of impurities on fluid properties and perform sensitivity studies (a "scoping" study to motivate future analyses);
- Lack of validation data.

Additional Remarks:

- The progress in thermal-hydraulic sub-channel modeling of advanced reactors is towards:
  - Development and implementation of models for improving accuracy of the predictions (including feedback parameters to neutronics):
    - Traditional mechanistic modeling approach could be efficiently supplemented/replaced by high-to-low model information approach and physics-informed data-driven modeling.
  - Acceleration and parallelization for improving efficiency of sub-channel core simulations especially on pin-resolved level.
  - The development and implementation of residual formulations of sub-channel codes will help to address both improving the efficiency and accuracy of sub-channel calculations as well as improving the coupling with neutronics codes towards fully implicit coupling.

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Thank you!

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Questions?