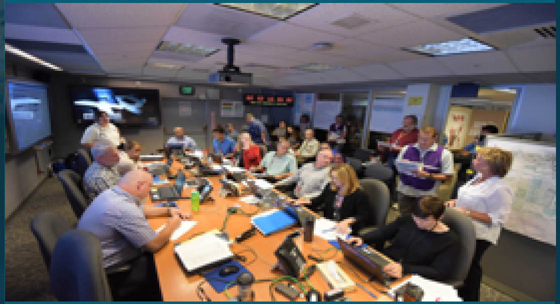
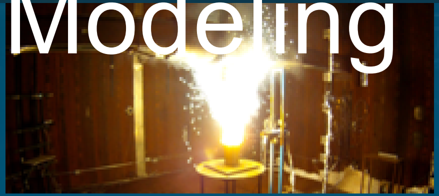
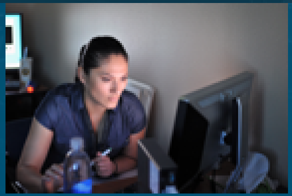
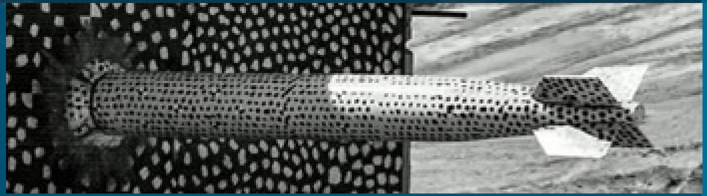
SAND2022-8113C

MELCOR for High Temperature Gas-cooled and Fluoride High Temperature Reactor Modeling









MELCOR Workshop
June 13-11, 2021

PRESENTED BY

Brad Beeny

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MELCOR HTGR and FHR Modeling and Development Thermal Hydraulics – Theory

Overview

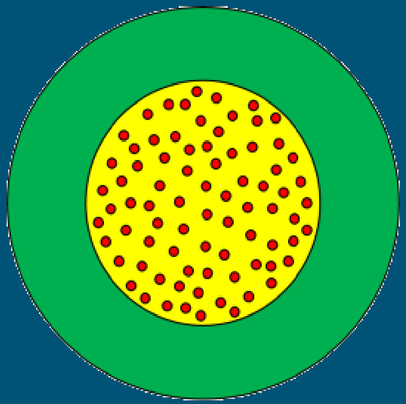
COR thermal hydraulics theory – generally applicable to both HTGRs and FHRs

- COR components and materials
  - Specialized MX and RF components for HTGR/FHR cores
  - Interpretation of FU for HTGR/FHR fuel elements
  - Specification of materials
  - Elements of best practice for components, materials, and nodalization
- Conduction
  - Intracell (between components within a COR cell)
  - Intercell (between components in adjacent COR cells)
  - Boundary (between COR and core boundary HS)
- Convection and flow
- Point Reactor Kinetics
- Oxidation (HTGR)
- Control volume hydrodynamics working fluid
- Other references

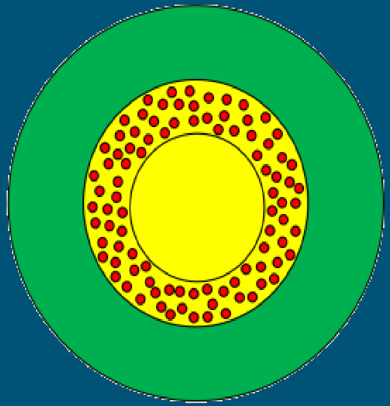
Conclusions

…COR Components and Materials…

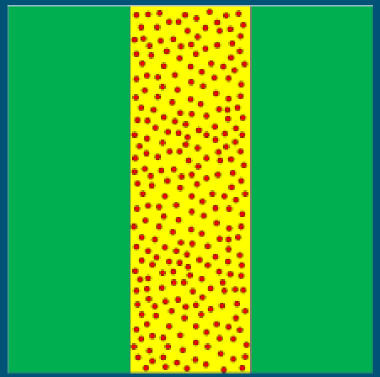
Conventional Pebble Fuel Element (HTGR/PBR)



Annular Pebble Fuel Element (FHR)



Prismatic Fuel Element (HTGR/PMR)



TRISO	Fuel (FU)
GRAPHITE	Fuel Extra Material (FUXM)
GRAPHITE	Matrix (MX)

COR Components – Matrix (MX)

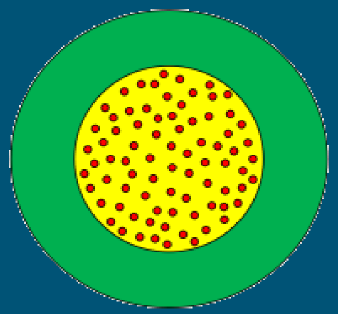
Matrix (MX) component is non-supporting, one-sided, and “thick” for purposes of heat transfer calculations

- Allocate material mass, component surface area, and other geometry
- Ties in to diffusional fission product release model
- Generally participates in conduction, convection, radiation, and oxidation

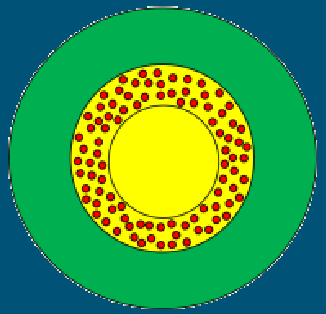
MX participates in intracell conduction (FU/MX) and intercell conduction (MX-MX, MX-RF, MX-SS)

MX is best pictured conceptually as the unfueled (TRISO free) region of a fuel element (green below)

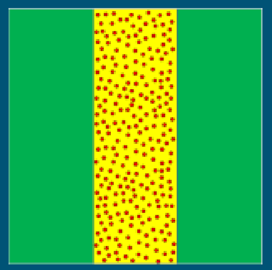
Conventional Pebble Fuel Element (HTGR/PBR)



Annular Pebble Fuel Element (FHR)



Prismatic Fuel Element (HTGR/PMR)



COR Components – Reflector (RF)

Reflector (RF) component is non-supporting, two-sided, and can have multiple orientations

- Radial reflectors (oriented inner/outer)
- Axial reflectors (oriented upper/lower)
- Generally participates in conduction, convection, radiation, and oxidation

RF participates in intercell conduction (RF-RF, RF-MX, RF-SS) and should not be collocated with FU and MX, rather it should be radially adjacent, e.g:

- Radially adjacent central reflector and active fuel region
- Radially adjacent peripheral/outer reflector and active fuel region

Core support logic:

- RF cannot bear the load of FU/MX above, e.g. a bottom reflector cannot “hold up” the active core
- FU/MX cannot bear the load of RF above, e.g. a top reflector cannot be “held up” by the active core
- Utilize SS (e.g. primary material GRAPH) where necessary and preferably in its own COR cells (not mixed with MX or RF)

COR Components – Fuel (FU) and Extra Material (FUXM)

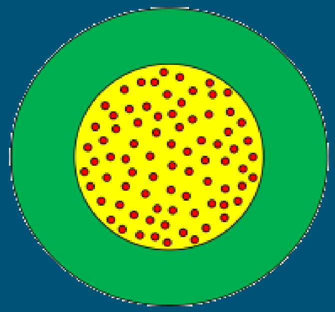
Fuel (FU) component is non-supporting, one-sided, and can include “extra material” (FUXM)

- Generally participates in conduction and radiation
- Ties to diffusional fission product release model and participates in radionuclide transport

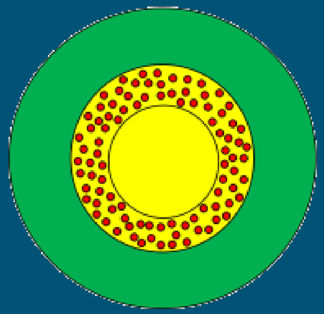
FU/FUXM participates in intracell conduction (FU/MX) and should be collocated with MX (like FU/CL in LWR)

FU/FUXM is best pictured conceptually as the fueled (TRISO laden) region of a fuel element (red/yellow below)

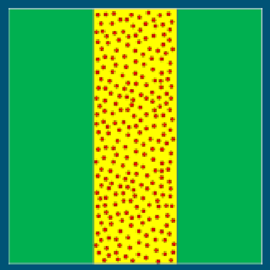
Conventional Pebble Fuel Element (HTGR/PBR)



Annular Pebble Fuel Element (FHR)



Prismatic Fuel Element (HTGR/PMR)



COR Components – Primary Materials

Recall “primary materials” are:

- The chief constituent material of a core component,
- Optionally specified by component (COR MELGEN input),
- NOT restricted to conventional built-ins known to MELCOR (MP package),
- Possibly characterized with the new user-defined materials (UDM) capability, and
- Possibly characterized with the new generic oxidation model (GOM) interfaced to UDM so as to:
  - Define oxidation reaction stoichiometry and energetics, or
  - Permit UDM access to built-in MELCOR graphite oxidation models by way of GOM

COR_FUM, COR_MXM, and COR_RFM cards specify FUXM, MX, and RF material names

Recall COR_NMAT specifies component-wise mass of UDM’s when leveraged as primary materials

COR Components – Best Practices for Components/Materials

FU uses UO_2 (modify in MP as necessary, e.g. to UCO) and is collocated in COR cells with MX

FUXM is a part of FU and uses either GRAPH (built-in or MP redefinition) or some UDM

- COR_FUM for FUXM material name/mnemonic
- COR_KFU has a slot for extra material mass specification by COR cell

MX ***MUST USE*** UDM/GOM, COR_MXM, and COR_NMAT (invoking MX) to either:

- Template (copy) built-in GRAPH and access built-in graphite oxidation models, or
- Define a new material dissimilar to built-in GRAPH along with a user-specified oxidation model

RF uses either GRAPH (built-in or MP redefinition) or some UDM

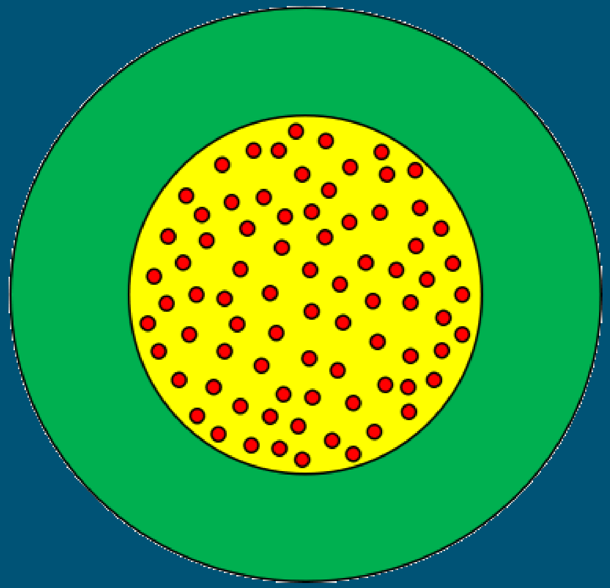
- COR_RFM for RF material name/mnemonic
- COR_KRF for material mass specification by COR cell
- COR_RFG to define orientation (cylindrical inner/outer, plate upper/lower)

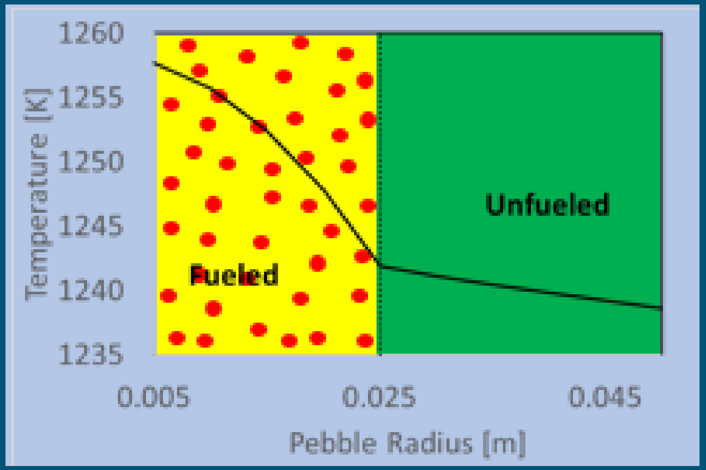
COR Components – Best Practices for Nodalization

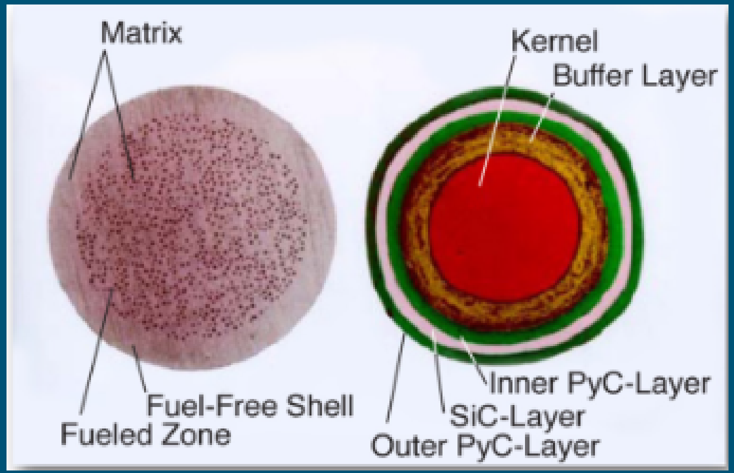
General guidelines:

- Use RF only in cells that comprise reflectors (besides SS graphite in cells for core support)
- Use FU and MX only in active core cells
- Use SS for actual core support structures
- Use SS on an as-needed basis to hold up FU/MX and/or RF and avoid support logic issues
- Component collocation:
  - Always collocate FU and MX,
  - Never collocate FU/MX and RF,
  - Never collocate FU/MX with SS, and
  - Avoid collocating RF and SS in an attempt to alleviate support logic issues

…Core Conduction…







COR Conduction – Intracell (FU/MX)

Intracell conduction between collocated FU and MX

- Account for FU conduction resistance and non-negligible MX conduction resistance
- Modify the FU-to-MX conductance in terms of its serial/parallel resistance combinations

$$q_{FU-to-MX} = h_{FU,MX} A_{FU} (T_{FU} - T_{MX})$$

$$\frac{1}{h_{FU,MX}} = \frac{1}{h_{FU}} + \frac{1}{\frac{1}{\frac{1}{h_{gap}} + \frac{1}{h_{CF}}} + h_{rad}} + \frac{1}{h_{MX}} \quad , \quad for \quad \frac{1}{h_{MX}} = \begin{cases} k_{MX} a / f R_{MX,i} & ,PMR \\ k_{MX} a / f R^2_{MX,i} & ,PBR \end{cases} \qquad 1/h_{FU} = \begin{cases} \frac{R_{FU}}{4k_{FU}} ,PMR \\ \frac{R_{FU}}{5k_{FU}} ,\text{PBR} \end{cases}$$

$$a = \begin{cases} \left(\ln\left(\frac{R_{MX,o}}{R_{MX,i}} \right) \right)^{-1} & ,PMR \\ \left(1/R_{MX,i} - 1/R_{MX,o} \right)^{-1} & ,PBR \end{cases}$$

$$f = \begin{cases} \left(\frac{1}{2} \right) \left(\frac{2R^2_{MX,o} \ln\left(\frac{R_{MX,o}}{R_{MX,i}} \right) - \left(R^2_{MX,o} - R^2_{MX,i} \right)}{\left(R^2_{MX,o} - R^2_{MX,i} \right) \ln\left(\frac{R_{MX,o}}{R_{MX,i}} \right)} \right) & ,PMR \\ \frac{1/R_{mx,i}}{1/R_{mx,i} - 1/R_{mx,o}} - \left(\frac{3/2}{1/R_{mx,i} - 1/R_{mx,o}} \right) \left(\frac{R^2_{mx,o} - R^2_{mx,i}}{R^3_{mx,o} - R^3_{mx,i}} \right) & ,PBR \end{cases}$$

Beeny, B.A. “Thermal Hydraulic Analysis of a Reduced Scale High Temperature Gas Cooled Reactor Test Facility and its Prototype with MELCOR“. MS Thesis, Texas A&M University, 2012

COR Conduction – Intercell

Intercell conduction (allows: MX-MX, MX-RF, RF-SS, MX-SS ; disallows: FU-FU for PBR)

- General equation (axial or radial):

$$q_{i,j} = K_{eff}\left(T_i - T_j\right)$$

- Effective conductivity K_{eff}:

$$K_{eff} = \frac{1}{{}^{1}/_{K_i} + {}^{1}/_{K_j}} \quad ; \quad K_i = \frac{k_i A_i}{\Delta x_i}$$

- For RF and SS
  - Conductivity k_i comes from solid thermal conductivity data
  - Conduction areas and lengths are derived from notions of cell volumes, lengths, boundary areas, etc.

- For MX ONLY
  - Conductivity k_i comes from effective conductivity models
  - Conduction areas and lengths are similarly defined
  - Cell MX component "height fraction" derived from volume ratio force to unity (no artificial degradation of radial heat transfer)

→ best practice COR SC1507 set > 0.0 (real kind)

COR Conduction – Intercell

PBR effective conductivity model (pebble bed conduction) applied to MX component exclusively

- Zehner-Schlunder-Bauer with Breitbach-Barthels modification to the radiation term
- Accounts for conduction through pebbles and through fluid plus radiation

$$k_{eff} = \left(1 - \sqrt{1-\varepsilon}\right)\varepsilon 4\sigma T^3 D_p + \left(1 - \sqrt{1-\varepsilon}\right)k_f + \sqrt{1-\varepsilon}\, k_c$$

$$k_c = \frac{2}{N}\left\{ \frac{B\left(1 + \frac{1}{\Lambda_s\left(\frac{2}{\varepsilon_r} - 1\right)} - \lambda\right)}{N^2 \frac{1}{k_f}} \ln\left(\frac{\lambda_p + \lambda_r}{B}\right) + \frac{B+1}{2B}\left(\frac{4\sigma T^3 D_p}{\frac{2}{\varepsilon_r} - 1} - Bk_f\right) - \frac{B-1}{N} k_f \right\}$$

$$\Lambda_s = \frac{k_s}{4\sigma T^3 D_p}$$

폭 ＝ 4σ퐽 팟

$$B = C\left(\frac{1-\varepsilon}{\varepsilon}\right)^m$$

C = 1.25
m = 10/9

$$N = 1 + \frac{1}{\left(\frac{2}{\varepsilon_r} - 1\right)\Lambda_s} - \lambda B$$

$\lambda = k_f/k_s$ $\lambda_P = k_s/k_f$ $\lambda_r = k_r/k_f$

* Same correlation with zeroed radiation components for FHR with FLiBe working fluid

COR Conduction – Intercell

PMR effective conductivity model (continuous solid with pores) applied to MX component exclusively
- Tanaka-Chisaka
- Accounts for solid conduction, pore conduction, and pore radiation
- A radiation term is incorporated into the pore (gas) conduction term
- After obtaining an effective PMR fuel element (hex block) conductivity, a parallel gap conductance term is added

$$k_{eff} = k_s \left[A + (1-A) \frac{\ln\left(1 + 2B\left(k_{por}/k_s - 1\right)\right)}{2B\left(1 - k_s/k_{por}\right)} \right]$$

$$k_{rad} = 4\varepsilon_r \sigma T^3 D$$

$$k_{por} = k_{s,por} + k_{rad}$$

$$k_{er} = \left({}^{1}/_{h_{gap} D_{blk}} + {}^{1}/_{k_{eff}} \right)^{-1}$$

k_{eff} = effective conductivity [W/m-K]
A = $2(1-\varepsilon)/(2+\varepsilon)$
B = $(1-\varepsilon)/3$
k_s = thermal conductivity of solid (continuous) material [W/m-K]
k_{por} = thermal conductivity of pores (discontinuous) material [W/m-K]
ε = porosity

h_{gap} = Gap heat transfer coefficient (W/m^2-K)
D_{blk} = Effective radial diameter of a block (m)

COR Conduction – Boundary

Boundary conduction occurs between COR components in the outermost ring and radial boundary HS's

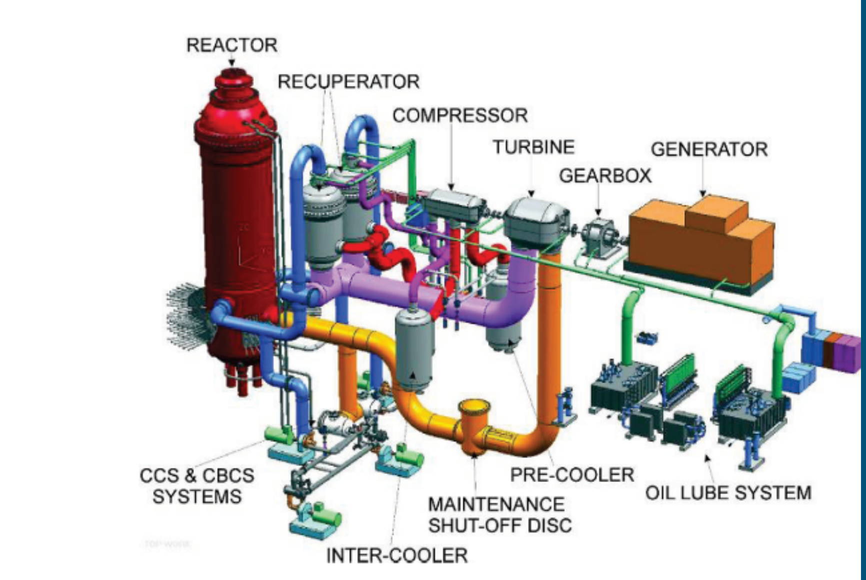
Governed by a contact resistance consisting of a gap component and a thermal diffusion component

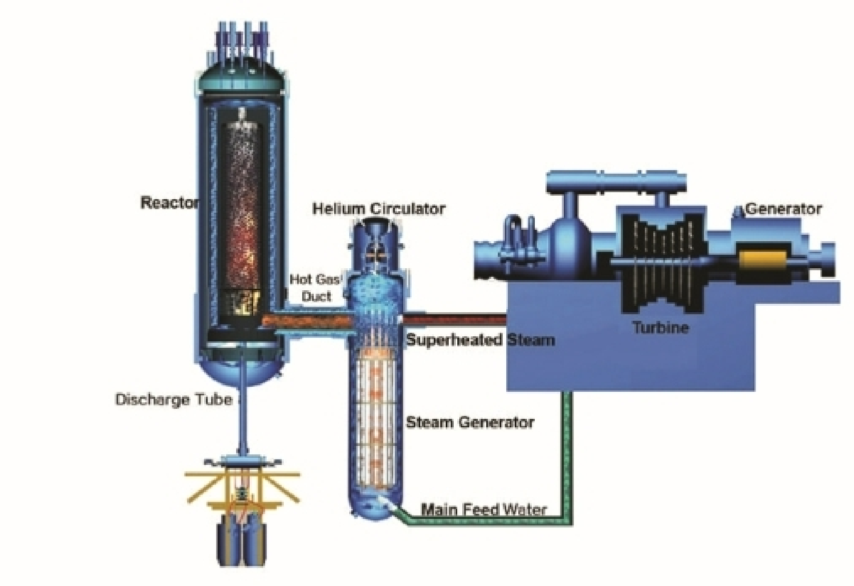
$$q_{C-HS} = \frac{T_C - T_{HS}}{R} \qquad R = R_{gap} + R_{dif} \qquad R_{gap} = \Delta r_{gap} / k_{gap} \qquad R_{dif} = \sqrt{\frac{\pi \Delta t}{(k \rho c_p)_{HS}}}$$

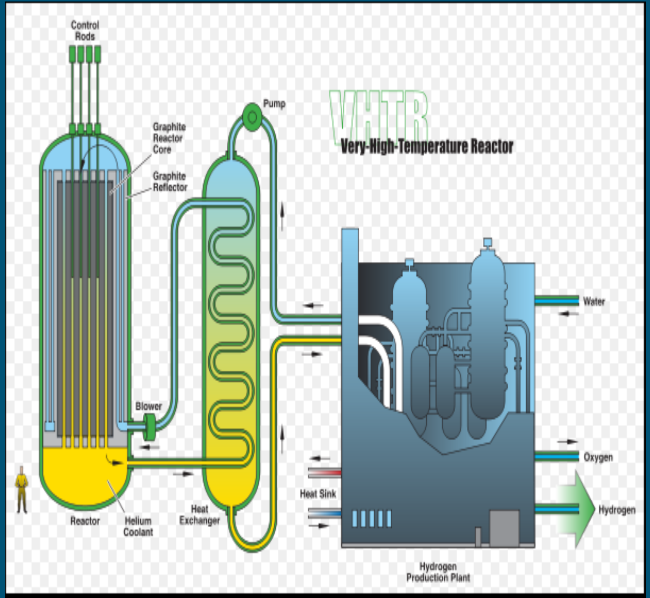
Thermal diffusion resistance mitigates oscillations due to explicit COR/HS coupling

As a best practice, use boundary conduction (COR_BCP) to allow energy transfer from the core periphery

…Core Convection, Point Kinetics, and Oxidation…







COR Convection – Heat Transfer

Heat transfer coefficient (Nusselt number) correlations for PBR

MX has a conduction component to it heat transfer resistance (parallel with convection term)

$$Nu = 2.0 + 0.6\ Re_f^{1/2}\ Pr_f^{1/3} \qquad Nu = 2.0 + 0.6\ Gr_f^{1/4}\ Pr_f^{1/3}$$

Isolated spherical particles
Film temperature to evaluate nondimensional numbers
Max of forced/free used

$$\frac{1}{h_{MX}} = \begin{cases} \dfrac{1-f}{k_{MX}\left({}^{a}/R_{MX,o}\right)} & ,PMR \\ \dfrac{1-f}{k_{MX}\left({}^{a}/R_{MX,o}^2\right)} & ,PBR \end{cases}$$

$$f = \begin{cases} \left(\frac{1}{2}\right)\left(\dfrac{2R_{MX,o}^2 \ln\left(\frac{R_{MX,o}}{R_{MX,i}}\right) - \left(R_{MX,o}^2 - R_{MX,i}^2\right)}{\left(R_{MX,o}^2 - R_{MX,i}^2\right)\ln\left(\frac{R_{MX,o}}{R_{MX,i}}\right)}\right) & ,PMR \\ \dfrac{{}^{1}/R_{mx,i}}{{}^{1}/R_{mx,i} - {}^{1}/R_{mx,o}} - \left(\dfrac{{}^{3}/_{2}}{{}^{1}/R_{mx,i} - {}^{1}/R_{mx,o}}\right)\left(\dfrac{R_{mx,o}^2 - R_{mx,i}^2}{R_{mx,o}^3 - R_{mx,i}^3}\right) & ,PBR \end{cases}$$

$$a = \begin{cases} \left(\ln\left(\frac{R_{MX,o}}{R_{MX,i}}\right)\right)^{-1} & ,PMR \\ \left({}^{1}/R_{MX,i} - {}^{1}/R_{MX,o}\right)^{-1} & ,PBR \end{cases}$$

COR Convection – Flow Resistance

Flow resistance due to packed bed flow as computed from one of several correlations (CVH SC4413)

- Ergun
- Modified Ergun (rough/smooth)
- Achenbach

Correlation	C_1	C_2	C_3	C_4
Ergun (original)	3.5	300.	0.0	-
Modified Ergun (smooth)	3.6	360.	0.0	-
Modified Ergun (rough)	8.0	360.	0.0	-
Achenbach	1.75	320.	20.0	0.4

K-loss formulation used in phasic velocity equations (CVH/FL)

$$K^* = K_{empty} + \left[C_1 + C_2 \frac{1-\varepsilon}{Re} + C_3 \left(\frac{1-\varepsilon}{Re} \right)^{C_4} \right] \frac{(1-\varepsilon)L}{\varepsilon D_p} \qquad Re = \frac{\rho\ \varepsilon\ v_j D_p}{\mu}$$

COR_ZP or COR_CPOR for porosities entering into packed bed K-loss calculations

Point Reactor Kinetics

Standard PRKE's with kinetics data accessible by sensitivity coefficient

Feedback models (Doppler, fuel/moderator density, external CF) and COR_TAVG for average temperatures

$$\frac{dP}{dt} = \left(\frac{\rho - \beta}{\Lambda}\right) P + \sum_{i=1}^{6} \lambda_i Y_i + S_0$$

$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P - \lambda_i C_i, \qquad for\ i = 1 \ldots 6$$

P= Thermal power due to fission

Y_i= Thermal power due to delayed neutron precursor group i

S_0= Thermal power generation rate due to neutron source

$\rho = \frac{k-1}{k}$= Reactivity for k the effective multiplication factor

β= Delayed neutron fraction

$\Lambda = {}^{1}/_{\nu V \Sigma_f}$= Neutron generation time

λ_i= Decay constant of delayed neutron precursor group i

Oxidation - HTGR

Steam oxidation

$$R_{OX,steam} = \frac{k_4 P_{H_2O}}{1 + k_5 P_{H_2}^{0.5} + k_6 P_{H_2O}}$$

Reaction	ΔH (kcal/mol)
$C + H_2O(g) \rightarrow CO(g) + H_2(g)$	+31.14
$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$	-9.65

where

$R_{OX,steam}$ = Reaction rate for steam oxidation [1/s]
P_{H_2O} = Partial pressure of H_2O [Pa]
P_{H_2} = Partial pressure of H_2 [Pa]
k_i = ith reaction coefficient = $K_i \exp\left(-\frac{E_i}{RT}\right)$
K_i = ith precoefficient
E_i = ith activation energy [J/kmol]
R = Gas constant = 8314 [J/kmol-K]
T = Temperature [K]

	K_i	E_i/R
k_4	$2.646\text{x}10^{-4}$ [1/s-Pa]	16455 K
k_5	$1.075\text{x}10^{-12}$ [1/$Pa^{1/2}$]	30596 K
k_6	$4.887\text{x}10^{-21}$ [1/Pa]	20129 K

Includes rate limit due to steam diffusion towards active oxidation surface

Oxidation - HTGR

Air oxidation

$$R_{OX} = 1.7804x10^4 \exp\left(-\frac{20129}{T}\right)\left(\frac{P}{0.21228x10^5}\right)^{0.5}$$

where

R_{OX} = Reaction rate [1/s],
T = Temperature [K],
P = Oxygen partial pressure [Pa].

Reaction	ΔH (kcal/mol)
1. $C + O_2 \rightarrow CO_2(g)$	-94.03
2. $C + \frac{1}{2}O_2 \rightarrow CO(g)$	-26.62
3. $CO(g) + \frac{1}{2}O_2(g) \rightarrow CO_2(g)$	-67.41
4. $C + CO_2(g) \rightarrow 2CO(g)$	+40.79

Includes rate limit as with steam oxidation

Two SC enhancements (catalysis, pore diffusion)
→ COR SC1014 and SC1015

Empirical CO-to-CO_2 ratio

$$f_{CO/CO_2} = 7396e^{-69604/RT}$$

where

f_{CO/CO_2} = CO/CO_2 mole ratio
R = Gas constant = 8.314 [J/mol-K]
T = Temperature [K]

CVH Working Fluid

For PBR, PMR, and FHR, the COR/CVH connections are configured as usual

PBR and PMR working fluid is helium

- Configure initial thermodynamic conditions in CVH
- NCG helium in an “atmosphere-only” scenario
- Require no working fluid EOS library files to access (NCG package facilitates)

FHR working fluid is FLiBe

- Configure initial thermodynamic conditions in CVH
- FLiBe in a “pool-only” scenario
- Require a working fluid EOS library file and a global input record (cover this in subsequent MSR presentations)

Other References

Note that the COR thermal hydraulics models used for PBR and/or PMR – the traditional HTGR reactor types – are equally applicable to other reactor types that use a different working fluid but the same fuel elements (e.g. FHR)

Recent useful references on related subject matter:

- SNL's USNRC source term demo calculation for HTGR (PBR) and FHR
- 2021 EMUG presentation on HTGR best practices
- 2022 EMUG and AMUG
- 2022 NURETH-19 materials

Conclusions

COR PBR/PMR thermal hydraulics theory/physics was reviewed in some detail and these concepts are generally applicable to the pebble fueled FHR reactor design

Elements of best practice were discussed

Key takeaways:

- Understand how to configure FU (FUXM), MX, RF, and SS plus how to connect primary materials (including UDMs)
- Understand the specialized MX component
- Understand some basic points about nodalizing a PBR, PMR, or FHR core in view of thermal hydraulics modeling