



MELCOR for High Temperature Gas-cooled Reactor Modeling



Asian MELCOR User Group November 8-11, 2021

PRESENTED BY

Sandia National Laboratories Technical Staff



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MELCOR HTGR
Modeling/Development
Thermal Hydraulics – Theory



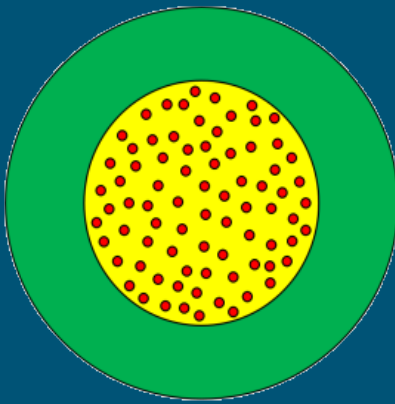
COR thermal hydraulics theory

- COR components and materials
 - Specialized MX and RF components for HTGR cores
 - Interpretation of FU for HTGR 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
- Other references

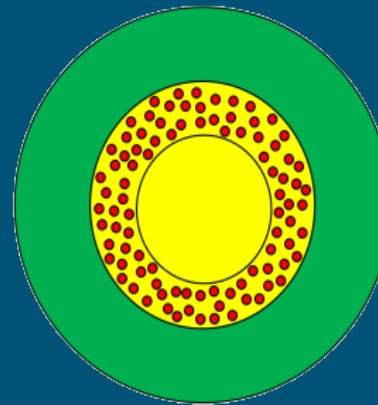
Conclusions

...COR Components and Materials...

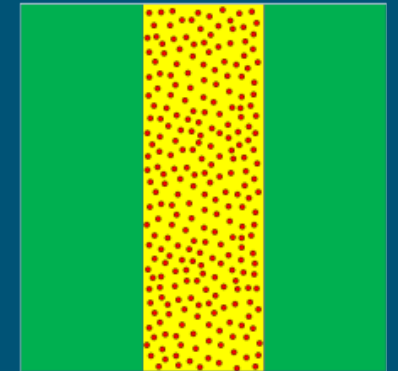
Conventional
Pebble Fuel
Element



Annular Pebble
Fuel Element



Prismatic Fuel
Element



TRISO

Fuel (FU)

GRAPHITE

Fuel Extra Material (FUXM)

GRAPHITE

Matrix (MX)

COR Components – Matrix (MX)



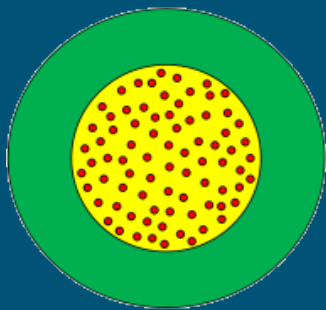
Matrix (MX) component is non-supporting, one-sided, and “thick” for purposes of heat transfer calculations

- 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

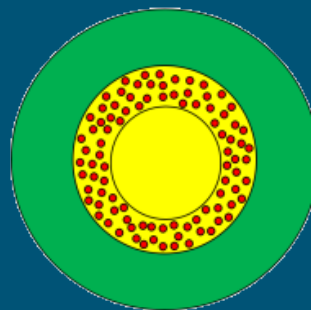
MX participates in intracell conduction (FU/MX) and intercell conduction (MX-MX, MX-RF, MX-SS)

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

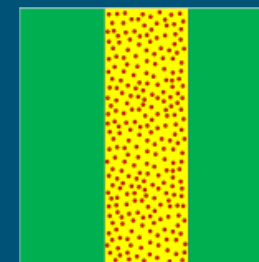
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COR Components – Reflector (RF)



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)

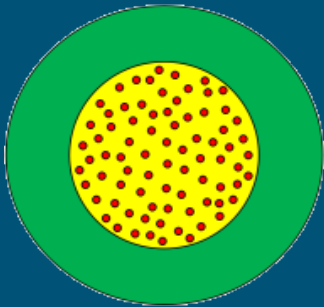
Fuel (FU) component is non-supporting, one-sided, and can include “extra material” (FUXM)

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

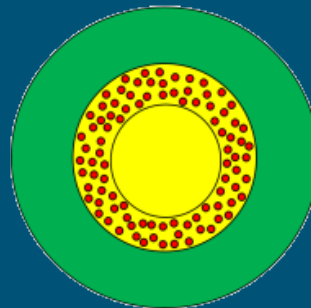
FU/FUXM participates in intracell conduction (FU/MX) and should be collocated with MX (like FU/CL in LWR)

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

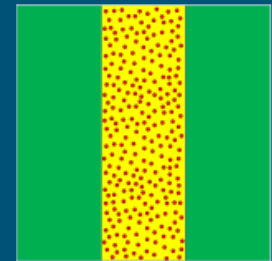
Conventional
Pebble Fuel
Element



Annular Pebble
Fuel Element



Prismatic Fuel
Element





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



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

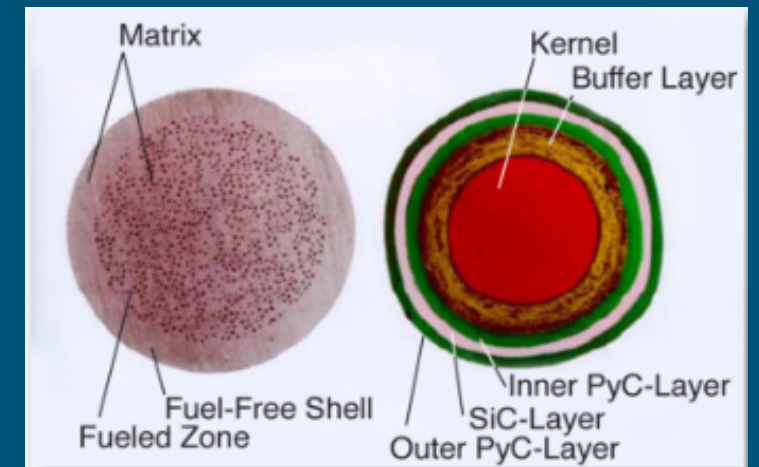
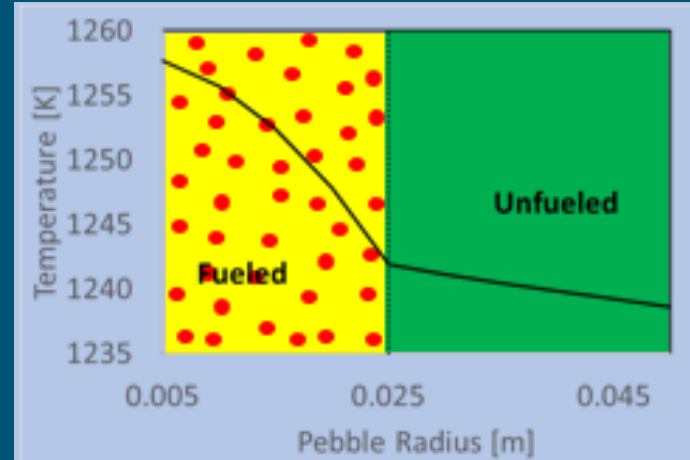
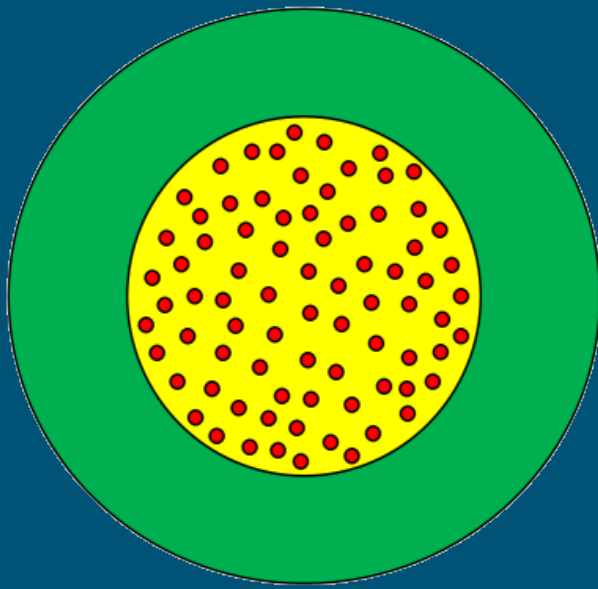
- COR_RFM for RF material name/mnemonic
- COR_KRF for material mass specification by COR cell
- COR_RFG to define orientation (cylindrical inner/outer, plate upper/lower)



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...





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

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

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

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



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

- General equation (axial or radial):

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

- 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)



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

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

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

$$\lambda = k_f/k_s \quad \lambda_p = k_s/k_f \quad \lambda_r = k_r/k_f$$

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

$$\text{푹푹} = 4\sigma \text{푹푹}$$

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

$$C = 1.25$$

$$m = 10/9$$

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



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

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

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

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

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

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/m²-K)

D_{blk} = Effective radial diameter of a block (m)



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

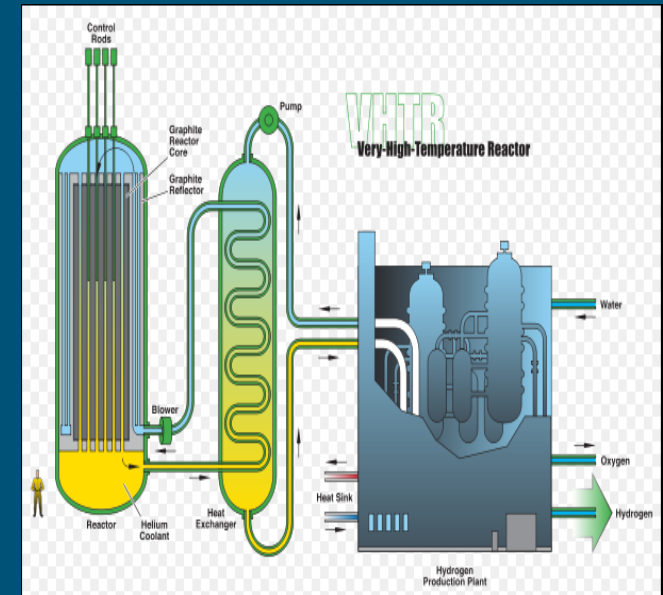
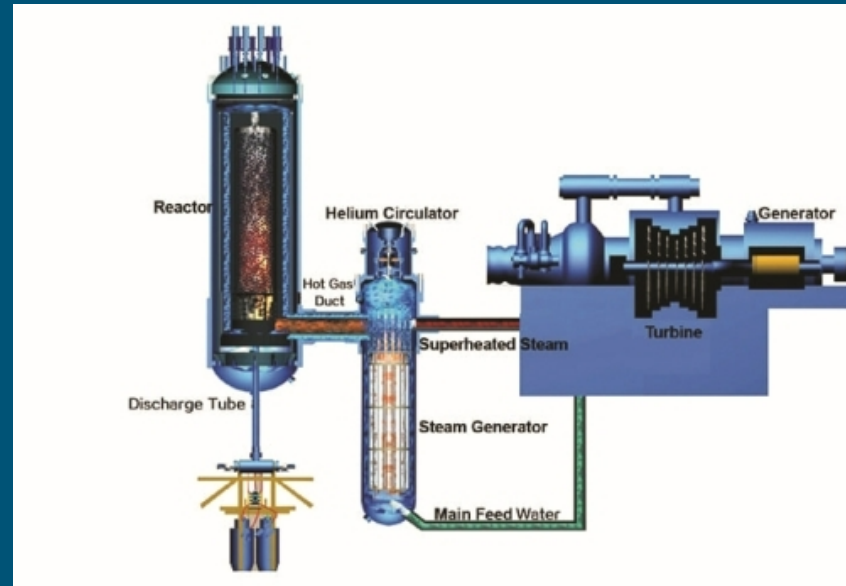
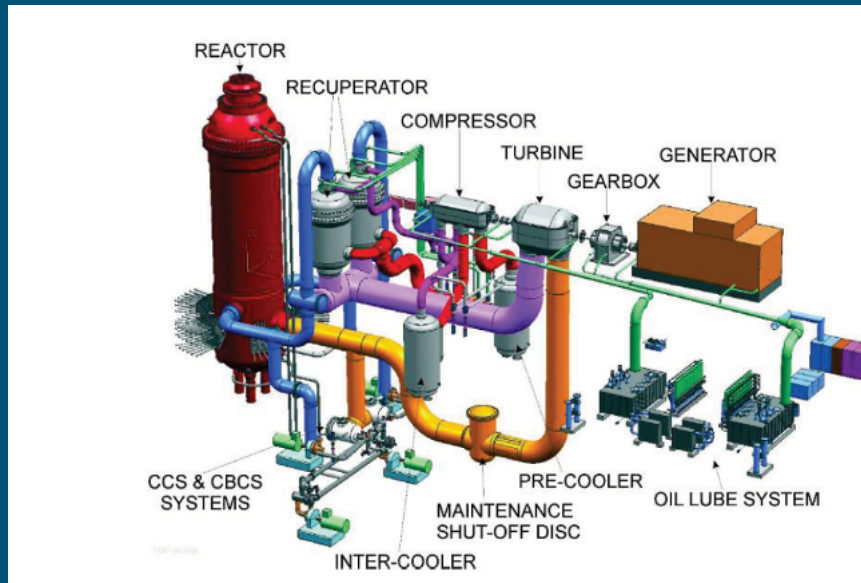
Governed by a contact resistance consisting of a gap component and a thermal diffusion component

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

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...





Heat transfer coefficient (Nusselt number) correlations for PBR

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

$$Nu = 2.0 + 0.6 Re_f^{1/2} Pr_f^{1/3}$$

$$Nu = 2.0 + 0.6 Gr_f^{1/4} Pr_f^{1/3}$$

Isolated spherical particles

Film temperature to evaluate nondimensional numbers

Max of forced/free used

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

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

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

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)

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

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

Standard PRKE's with kinetics data accessible by sensitivity coefficient

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

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

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

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

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	2.646×10^{-4} [1/s-Pa]	16455 K
k_5	1.075×10^{-12} [1/Pa ^{1/2}]	30596 K
k_6	4.887×10^{-21} [1/Pa]	20129 K

Includes rate limit due to steam diffusion towards active oxidation surface



Air oxidation

$$R_{OX} = 1.7804 \times 10^4 \exp\left(-\frac{20129}{T}\right) \left(\frac{P}{0.21228 \times 10^5}\right)^{0.5}$$

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

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

where

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



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)

Two recent and useful references on related subject matter:

- SNL's USNRC source term demo calculation for HTGR (PBR)
- 2021 EMUG presentation on HTGR best practices



COR PBR/PMR thermal hydraulics theory/physics was reviewed in some detail

Elements of best practice were discussed (refer to EMUG 2021 HTGR modeling best practices presentation)

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 or PMR core in view of thermal hydraulics modeling