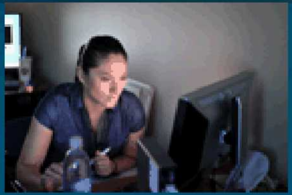
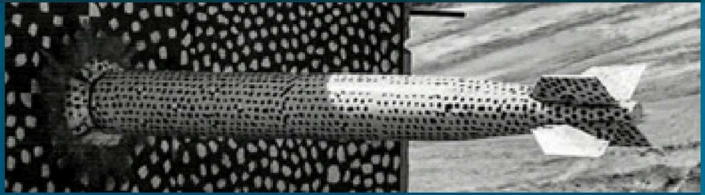
SAND2020-9480PE

MELCOR Overview and General Oxidation Model: ATF (FeCrAl)





Presented By:

Jesse Phillips

ATF PIRT Meeting September 2020

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Outline

Overview of MELCOR

- Historical Purpose
- Research Code
- General Functionality

Overview of the General Oxidation Model (GOM) and FeCrAl

- User-Defined Materials and Material Property Templating
- GOM Functionality

Purpose

NRC sponsored simulation code for analysis of accidents in nuclear power plants

- Conceived (in early 1980s) as a PRA (Probabilistic Risk Assessment) Code for LWRs (Light Water Reactors)
  - Primary objective: include consistent modeling of "all" relevant phenomena, including coupling of effects
- Application has expanded over the years
  - Other accidents, including DBA (Design Basis Accident) and containment response
  - Other reactor types, including heavy water reactors, heat pipe reactors, high temperature gas reactors, etc.
- Also used for various non-reactor analyses
  - General thermohydraulics model
  - Tracking transport of vapors or aerosol

Main phenomena modeled include

- Two-phase hydrodynamics, from RCS (Reactor Coolant System) to environment
- Heat conduction in solid structures
- Reactor core heatup and degradation
- Ex-vessel behavior of core debris
- Fission product release and transport
- Aerosol and vapor physics

Functionality

Three general building blocks

- Control volumes
- Flow paths
- Heat structures

Three specific modeling features

- Core structures
- Aerosol and fission product gas
- Molten core concrete

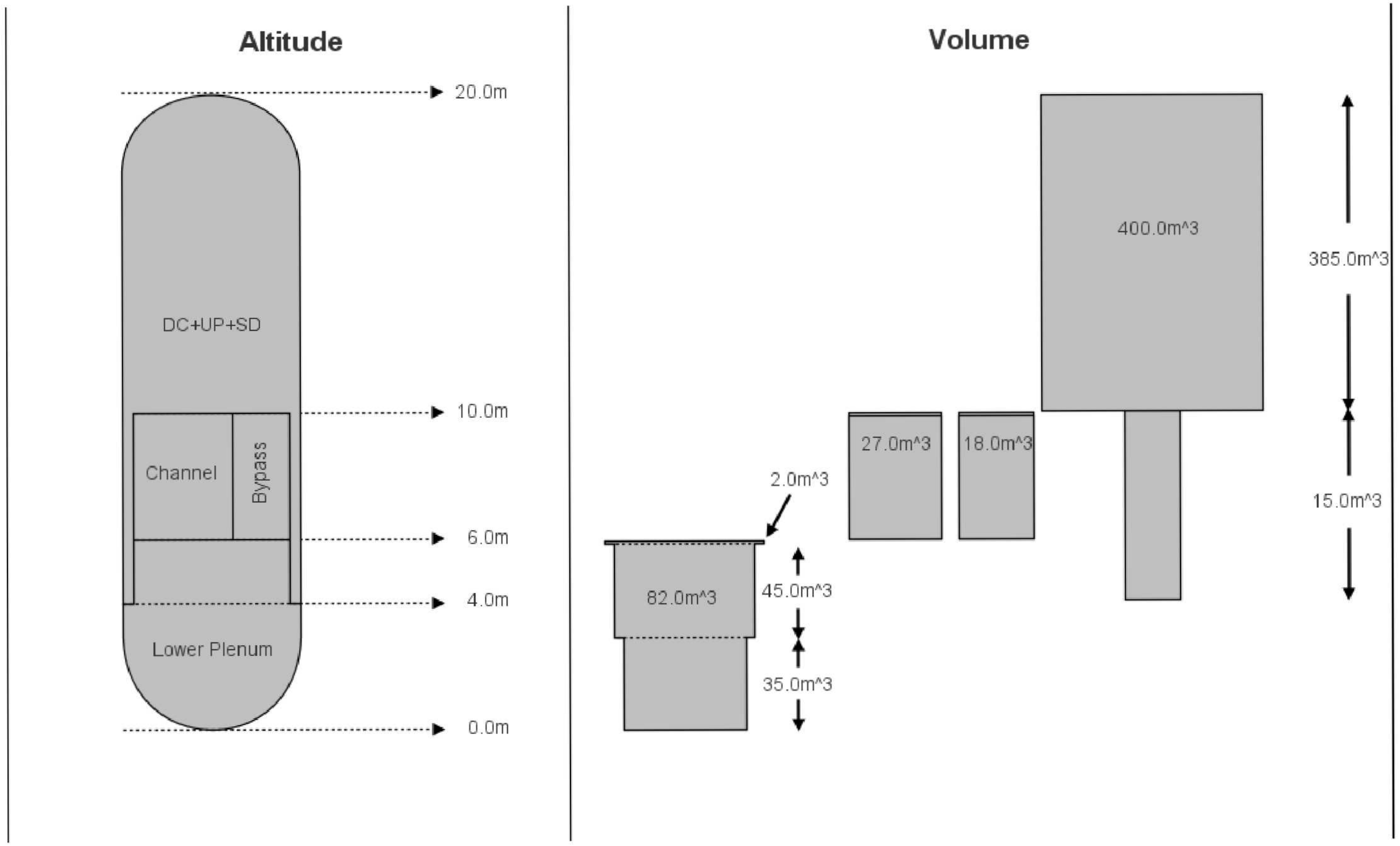
Functionality – Control volumes

Three general building blocks

- **Control volumes**
  - Arbitrary regions of space
  - Defined by
    - Basic Equation of States and state parameters
    - Free volume between specific altitudes
    - Initial fluid mass and energy
    - Heat and mass transfer at pool surface
    - Imposed gravitation separation of liquid water gases
- Flow paths
- Heat structures

Three specific modeling features

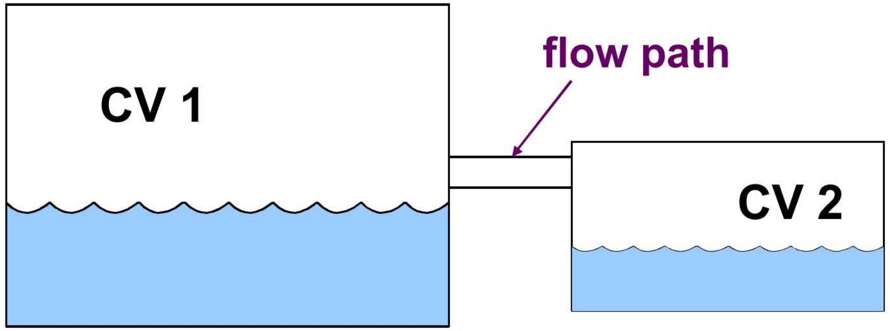
- Core structures
- Aerosol and fission product gas
- Molten core concrete

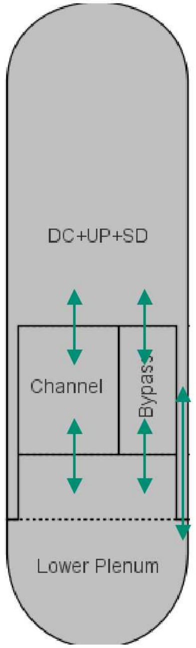


Functionality – Flow paths

Three general building blocks

- Control Volumes
- **Flow paths**
  - Separate momentum expression for liquid and atm.
  - Interphase for advection of fluids between two control volumes.
  - Provides friction characteristics, minor losses, exchange altitudes and open area
  - Flow path velocities are computed such that pressure predictions are resolved
- Heat structures





Three specific modeling features

- Core structures
- Aerosol and fission product gas
- Molten core concrete

Functionality – Heat structures

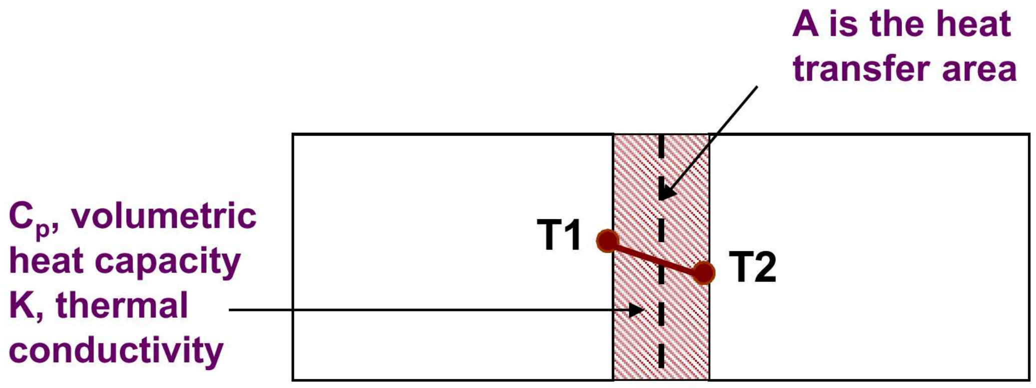
$$C_p \frac{\partial T}{\partial t} = \frac{1}{A}\frac{\partial}{\partial x}\left(KA\frac{\partial T}{\partial x}\right) + U$$

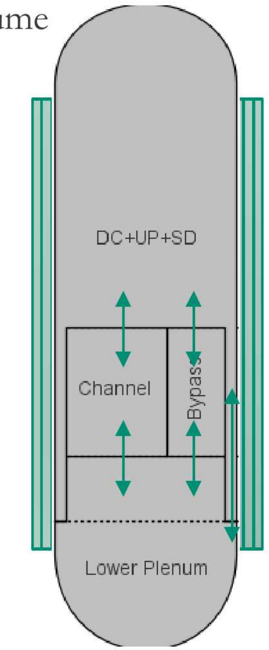
Three general building blocks

- Control Volumes
- Flow paths
- **Heat structures**
  - Models thermal response and mass/energy transfer to solid objects.
  - Compute 1D conduction internal to a given heat structure
  - Convection and radiation heat transfer to the surface of the structure from a control volume
  - Permits film transport across structure or deposited to a control volume
  - Deposition surface for aerosols

Three specific modeling features

- Core structures
- Aerosol and fission product gas
- Molten core concrete

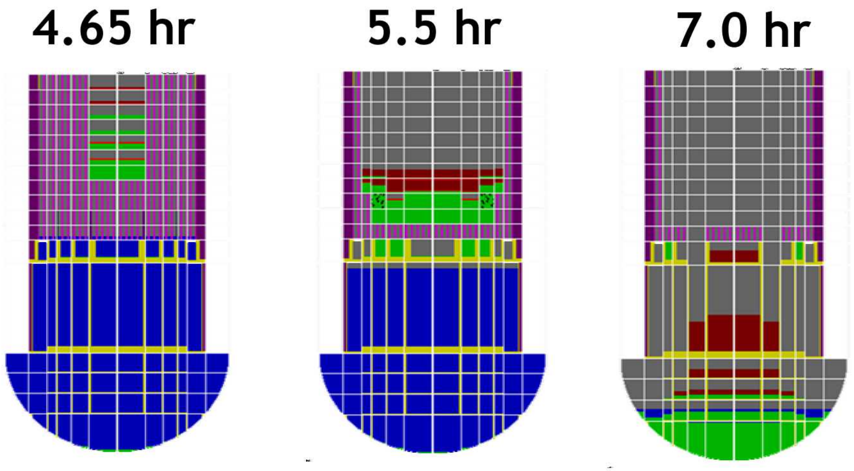


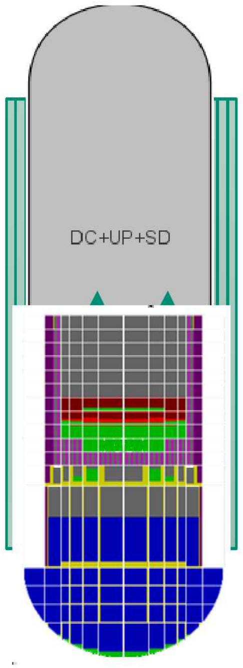


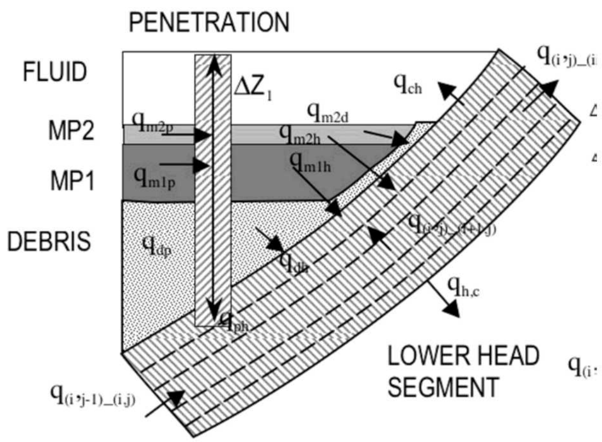
Functionality – Core structures

Three general building blocks
- Control Volumes
- Flow paths
- Heat structures

Three specific modeling features
- **Core structures**
  - Models internal structure of the core
  - Fluid boundary conditions are taken from associated control volume
  - Heat transfer, oxidation, clad failure, candling, material interaction, degradation, debris fields, molten pool formation, radiative losses
  - Lower head heat-up, failure mechanisms, penetrations, 2D conduction, melt and debris ejection
- Aerosol and fission product gas
- Molten core concrete

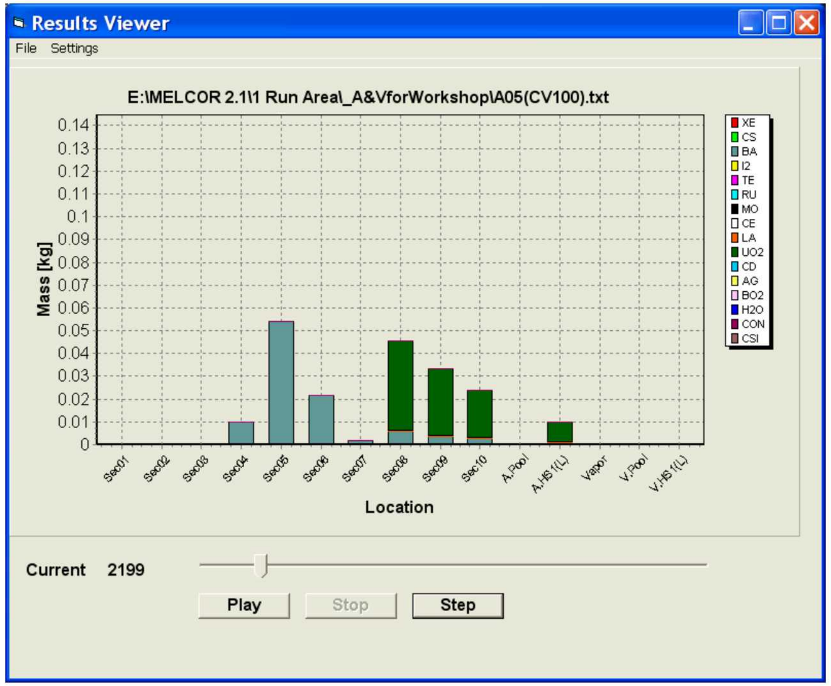






Curved Lower Head

Functionality – Core structures



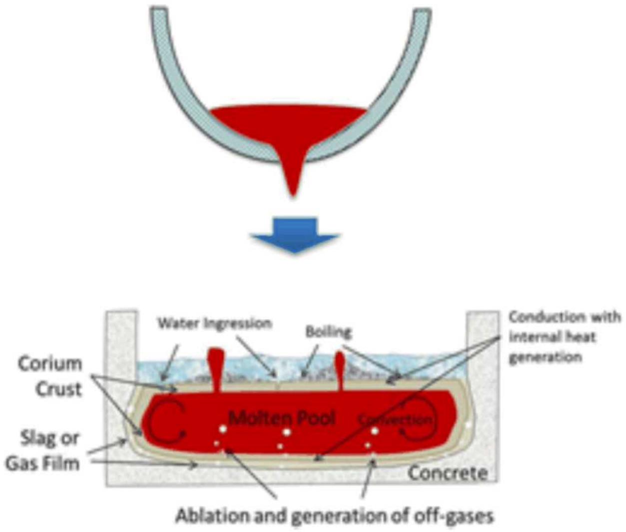
Three general building blocks

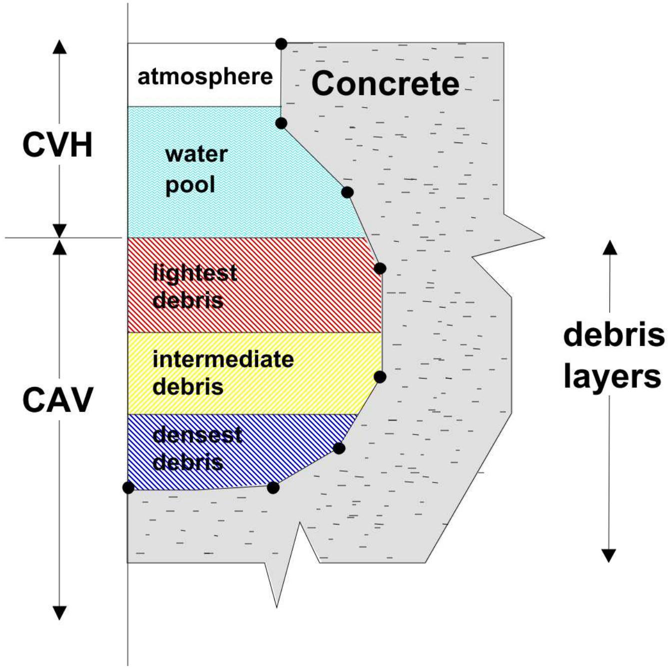
- Control Volumes
- Flow paths
- Heat structures

Three specific modeling features

- Core structures
- **Aerosol and fission product gas**
  - Models aerosol and fission product gas transport
  - Models apply representative element for all associated elements in a 'Class'
  - Assumed well-mixed in a given volume.
  - Fuel release modeling
  - Agglomeration and deposition of aerosols, condensation/vaporization to/from heat structure and aerosol surfaces
  - Discrete size distribution of aerosols in given control volume, but only tracks pregrouped elements with a single size distribution
  - Treated as trace elements which are advected given the volume fraction of control volume hydrodynamic material transport through flow paths
- Molten core concrete

Functionality – Core structures





Three general building blocks

- Control Volumes
- Flow paths
- Heat structures

Three specific modeling features

- Core structures
- Aerosol and fission product gas
- **Molten core concrete**
  - Compressed cylindrical melt model
  - Multi-node, centrally radiating track concrete surface evolution
  - Structural material added to melt, chemical reactions (including fission products), gas scrubbing and suspension of fission products, slag formation, gas film formation, etc.
  - Permits multiple layers for oxide/metal segregation (if desired), mixing, heat transfer
  - Doesn't compute heat transfer at temperature below the ablation temperature to the concrete
  - Does interact with overlying pool if present.

Material modeling for ATFs

User-defined Materials and a relaxation of prior MELCOR restraints

- Default material properties can be templated onto new materials
- Can be defined for COR with extra input
  - Emissivity, Viscosity, Thermal expansion coefficient, Oxidation behavior
  - Core behaviors are now exposed to users at a higher degree.

COR Component Primary Material

- Definition: surface-area dominant material of a component in its unoxidized state
- Determines which material, when multiple exist, oxidizes.
- Zr, SS, COR-USER-METAL have implicit oxides ZrO2, SSOX, COR-USER-OXIDE
- By default, if a component has only one material, it is the primary material.

Allow replacement of default materials as the dominant component material

- Example: replace Zircaloy in cladding component with another material
- COR UDMs can be assigned as Primary Materials

For multiple materials in a component, primary needs explicit assignment

- Example, cladding is a mixture of ZR and NUZR (previous slide)

General Oxidation Model (GOM)

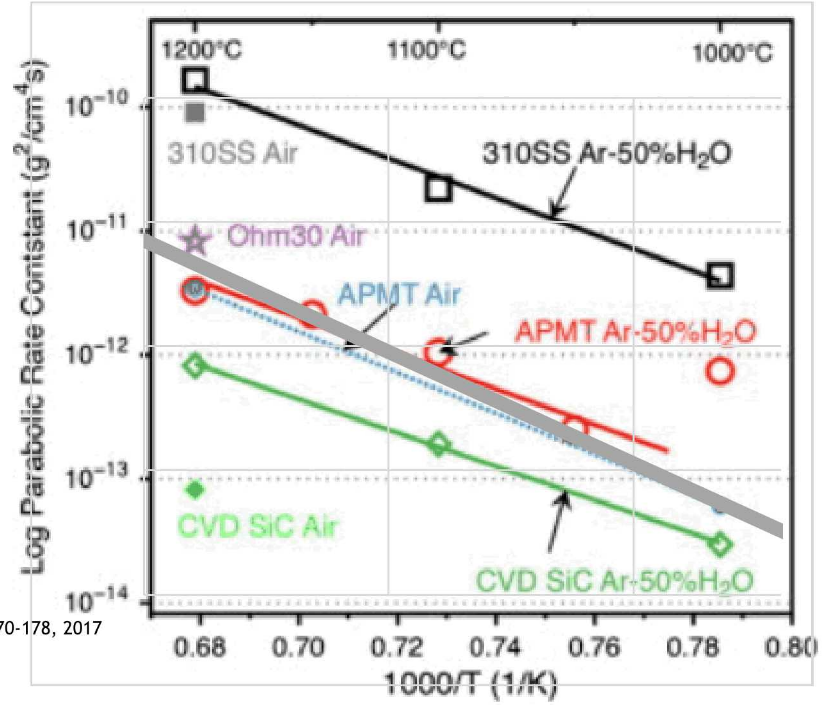
Oxidation has been generalized to make it more extensible for new materials

- Material database has been extended through User-Defined Materials are oxidizable.
- The general model applies the diffusion limited, parabolic rate equation for mass reacted expressed by weight gain.
- GOM permits direct specification of constants n, A, and B to fit specific material.
- Figure to the right present Pint et. al., experimental data and the fit provided by Robb, et.al. for mass gain for FeCrAl.
- However, MELCOR requires the coefficient, A, to be converted to mass of meta reacted.

$$\frac{dW^n}{dt} = K(T)$$

$$K(T) = Ae^{\frac{-B}{T}}$$

K(T) = 7.84 exp (-41376/T)



Merrill, B.J., Bragg-Sitton, S.M., Humrickhouse, P.W., Modification of MELCOR for Severe Accident Analysis of Candidate Accident Tolerant Cladding Materials, Nuclear Engineering and Design 315 170-178, 2017
K.R. Robb, H. Howell, and L.J. Ott, "Design and Analysis of Oxidation Tests to Inform FeCrAl ATF Severe Accident Models", Oak Ridge National Laboratory, ORNL/SPR-2018/893 (July 2018).
B.A. Pint, et al., "High Temperature Oxidation of Fuel Cladding Candidate Materials in Steam-Hydrogen Environments," Journal of Nuclear Materials 440, pp. 420-427, 2013.

General Oxidation Model (GOM)

GOM

- For a general reaction

Material + Oxidant => Oxide + H2 + CO + CO2 + CH4

Where, Oxidant may be either Steam or O_2

$$Mat + n\ H_2O \Rightarrow y\ MatOx + m\ H_2 + o\ CO + p\ CO_2 + qCH_4$$

Mol constants are user defined with the exception of m,
m is disregarded, instead a mass balance is performed for to compute the Hydrogen generation

$$\frac{dW^n}{dt} = K(T)$$

$$K(T) = Ae^{\frac{-B}{T}}$$

- Multiple reactions fraction of material interacting may be modeled

$$Mat + (n_i\ H_2O)\ X_i \Rightarrow\ (y_i MatOx + o_i\ CO + p_i CO_2 + q_i CH_4)\ Y_i$$

Where, X and Y are scalars values for reactants and products but are global constants at this time.

$$FeCrAl + (n_{Fe}\ H_2O)\ X_{Fe} \Rightarrow\ (y_{Fe} FeCrAl\_Ox + o_{Fe}\ CO + p_{Fe} CO_2 + q_{Fe} CH_4)\ Y_{Fe}$$

$$FeCrAl + (n_{Cr}\ H_2O)\ X_{Cr} \Rightarrow\ (y_{Cr} FeCrAl\_Ox + o_{Cr}\ CO + p_{Cr} CO_2 + q_{Cr} CH_4)\ Y_{Cr}$$

$$FeCrAl + (n_{Al}\ H_2O)\ X_{Al} \Rightarrow\ (y_{Al} FeCrAl\_Ox + o_{Al}\ CO + p_{Al} CO_2 + q_{Al} CH_4)\ Y_{Al}$$

→ Fe_1

→ Fe_2

→ …

General Oxidation Model (GOM)

GOM

- For each ith reaction unique A and B constants and multiple Temperature regions may be defined:

$$Mat + (n_i\ H_2O)\ X_i \Rightarrow\ (y_i MatOx + o_i\ CO + p_i CO_2 + q_i CH_4)\ Y_i$$

For jth temperature regions, given T

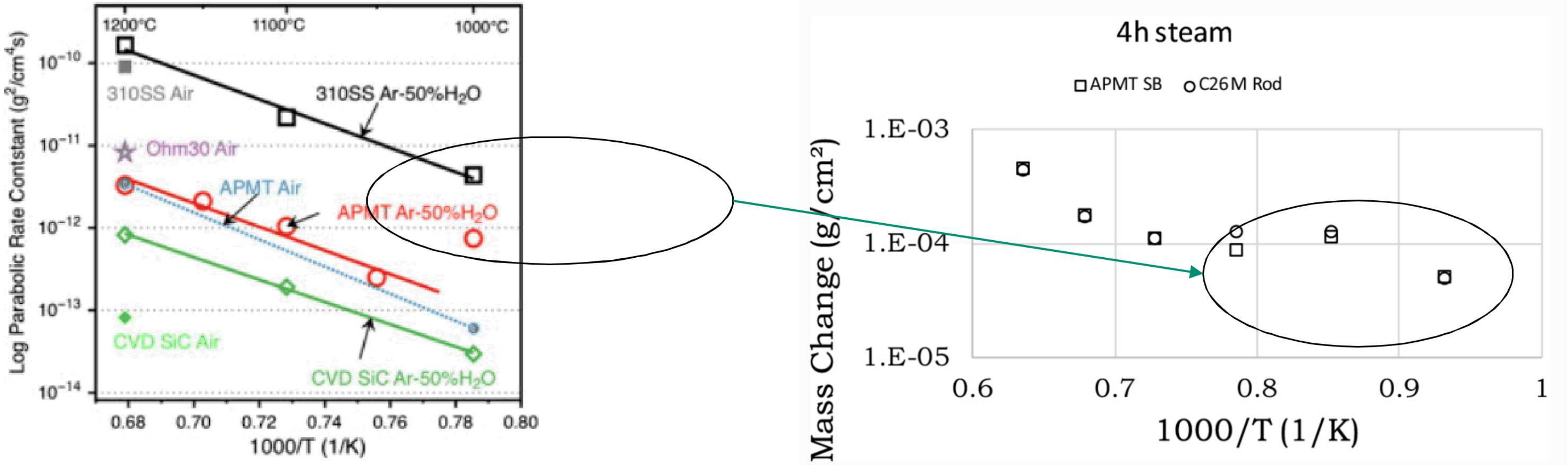
$T_{j-1} < T < T_j$: unique A_j, B_j, n_j

Allows variations in oxidation rates beyond the traditional breakaway.

Intent of the figures below is to show low temperature oxidation requiring more detailed temperature zones than the original two temperature zone

$$\frac{dW^n}{dt} = K(T)$$

$$K(T) = Ae^{\frac{-B}{T}}$$



Bebak, R.B., Gupta V.K., and Larson, M., Oxidation Characteristics of Two FeCrAl Alloys in Air and Steam from 800C to 1300C, Nuclear Materials, Oxidation, Supercritical CO2, and Corrosion Behavior, 2018

Conclusion

Known Limitations

- MELCOR transitions bulk material into oxide material.
  - There are not unique materials for tracking various oxide build up for detailed chemical reactions or varying protective effects of oxide formation.
  - FeCrAl -> FeCrAl-Oxide
- Only 5 oxidizable materials are available in total. Zr, Al, Stainless steel, Graphite, and one user-defined material.
  - All oxidizable materials can be modified to represent different materials by overwriting by the user, Zr -> new material with new oxidation parameters and core behavior.
- Likely more to be found throughout the PIRT process