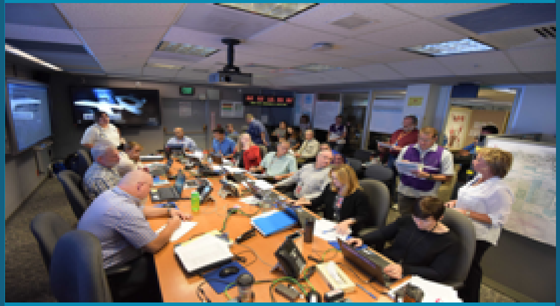
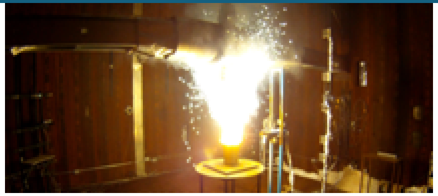
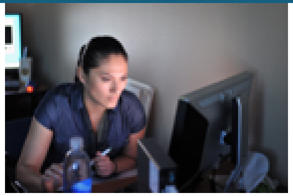
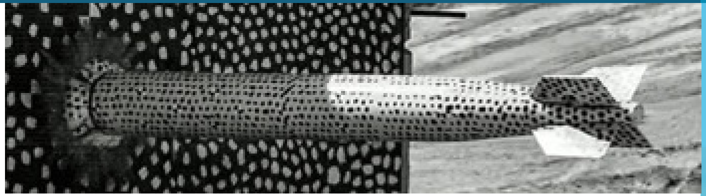
SAND2021-8327PE

MELCOR Development for New Nuclear Material Systems









David L. Luxat

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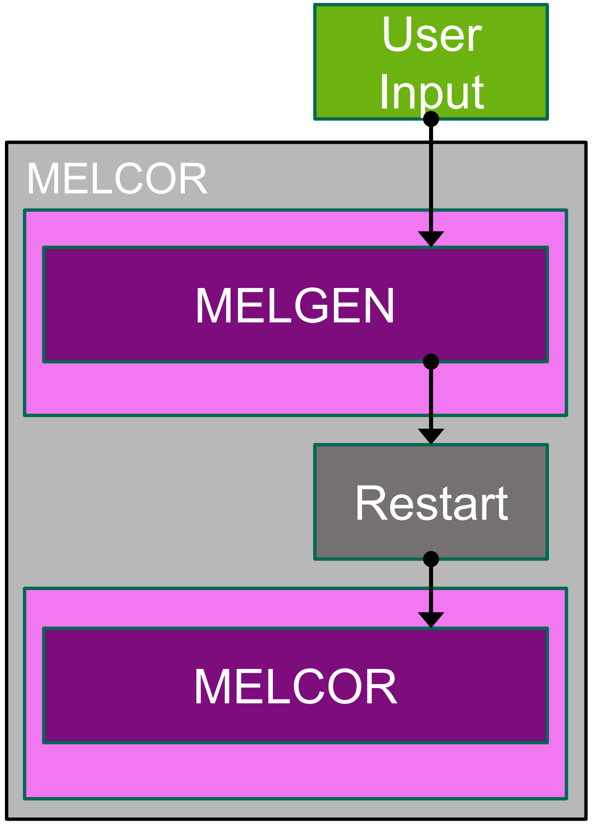
MELCOR Code System

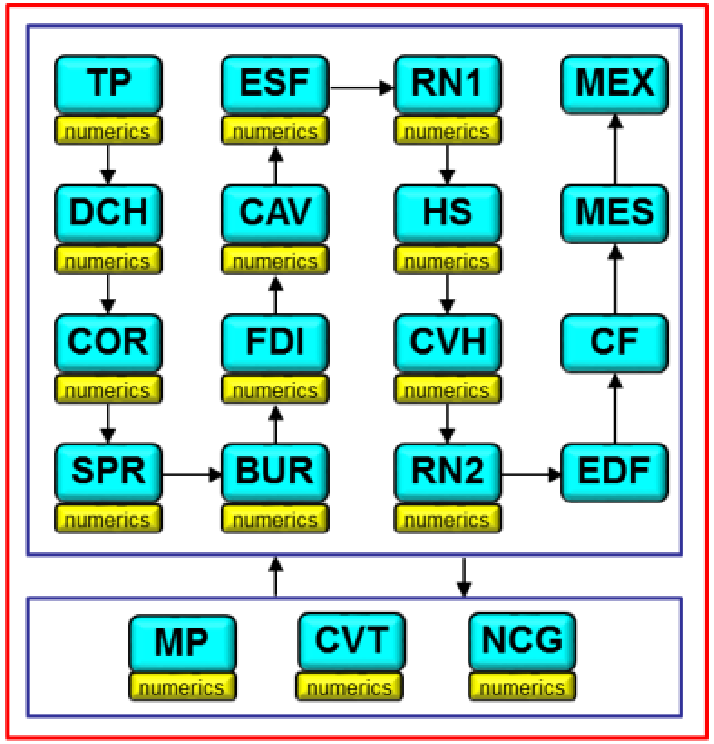
MELGEN
- User input processing
- Package activation
- Database setup
- Restart generation

MELCOR
- Evaluation of models
- Advancement of simulation through time

MELGEN used to initialize the simulation

MELCOR acts to evolve the state of the system stored into the database
- Evolves from an initial time with state present in restart file
- Evolution proceeds until specified end time of simulation





TP = Transfer Process
DCH = Decay Heat
COR = Core
SPR = Containment Spray
BUR = Gas Combustion
FDI = Fuel Dispersal Interaction
CAV = Cavity (MCCI)
ESF = Engineered Safety Features
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RN = Radionuclide
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Complexity and Accident Modeling

Equations encountered across MELCOR involve rate of change of some state with time

Complexity of modeling arises because of dynamic manner in which states coupled

- Prior to accident many interactions between "states" do not exist
- For example, fuel mass cannot be transported to chemically interact with cladding

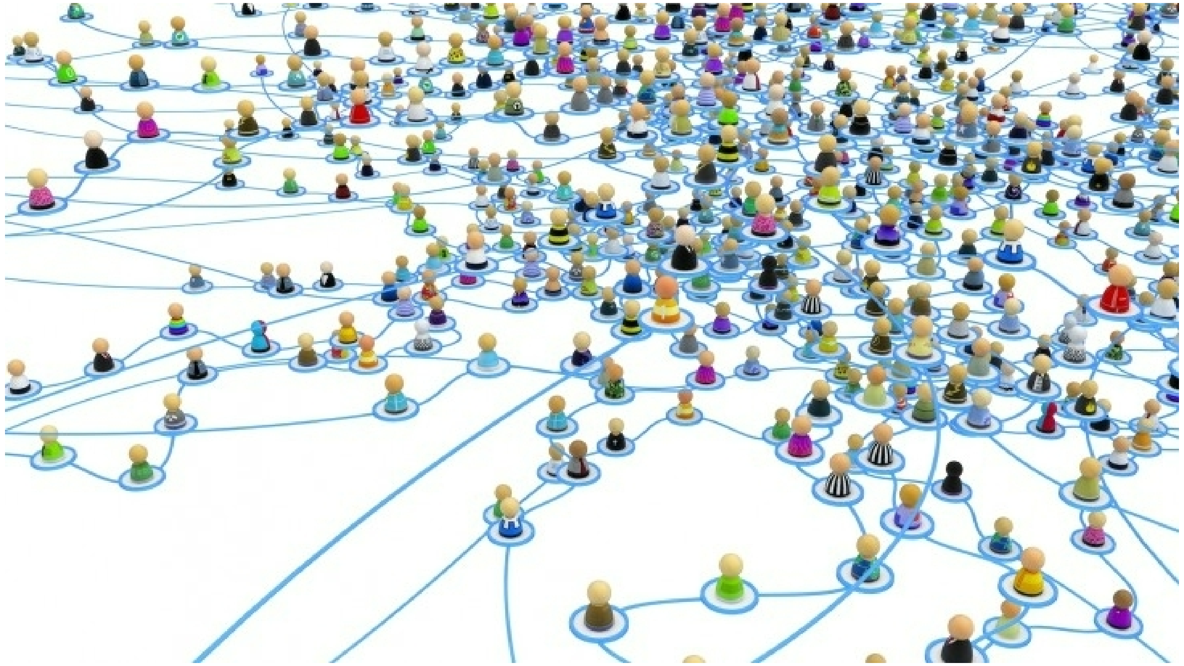
Process of core degradation exhibits features of combinatorial evolution

- With time, increasingly more degrees of freedom are liberated

Current models for many processes can be reduced to canonical form

$$\frac{d\boldsymbol{\sigma}}{dt} = \widehat{\mathcal{M}}(\boldsymbol{\sigma}, t)$$

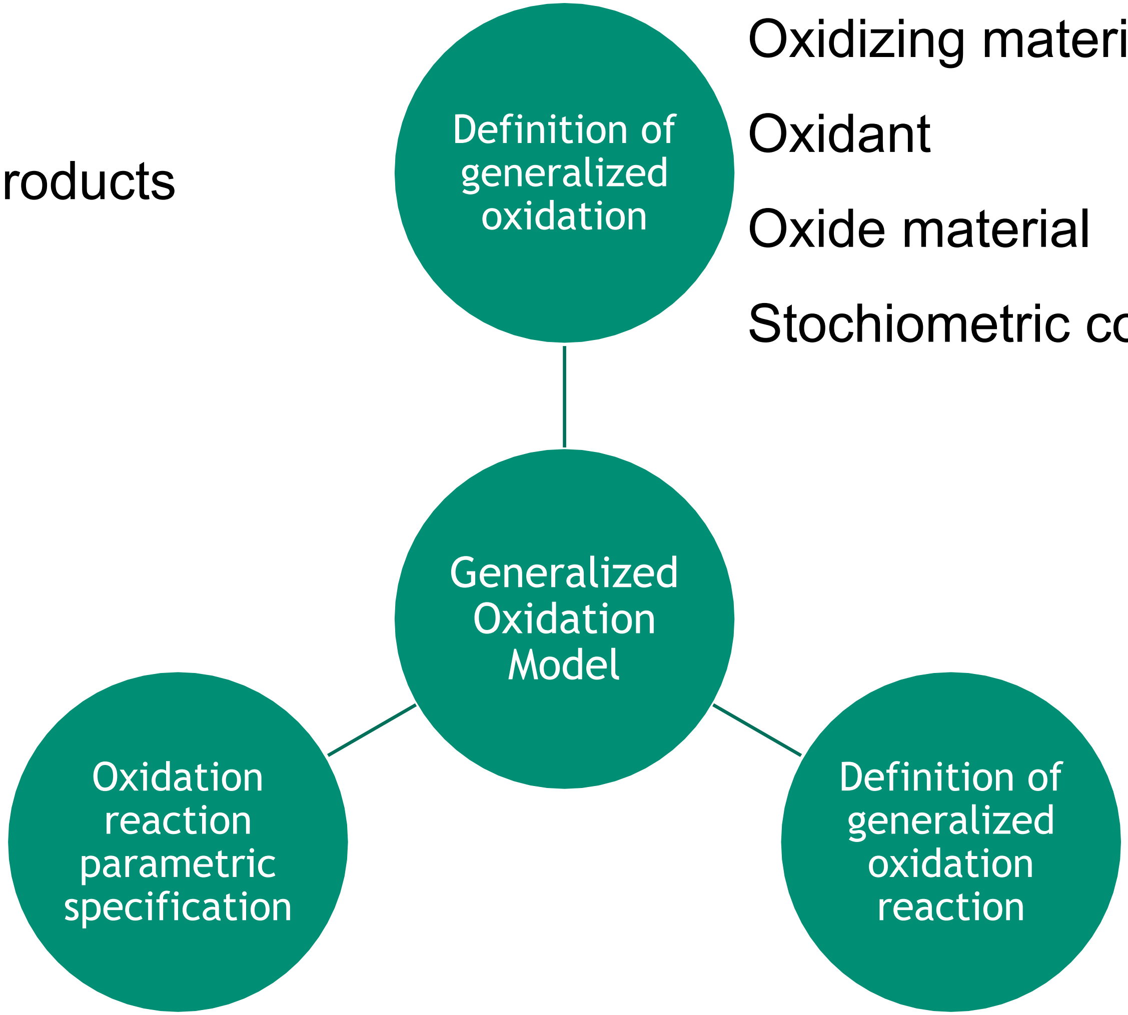
$$\frac{d\widehat{\mathcal{M}}}{dt} = \hat{\mathcal{F}}(\widehat{\mathcal{M}}, \boldsymbol{\sigma}, t)$$



Generalized Oxidation Model

Support for multiple oxide products introduced in generalized architecture

Arrhenius kinetics parameters



Oxidizing material

Oxidant

Oxide material

Stochiometric coefficients

$$\frac{d(W^n)}{dt} = A \exp\left(\frac{B}{T}\right)$$

MELCOR Molten Salt Model (MSM)

MELCOR provides mass of radionuclides released into salt, chemistry, T and P

→

MSM computes what remains in salt as soluble, colloidal, deposited, and released as vapor and aerosol

→

MELCOR continues to transport materials to and from the salt control volume

For Each Timestep

Molten Salt Fission Product Transport Modeling

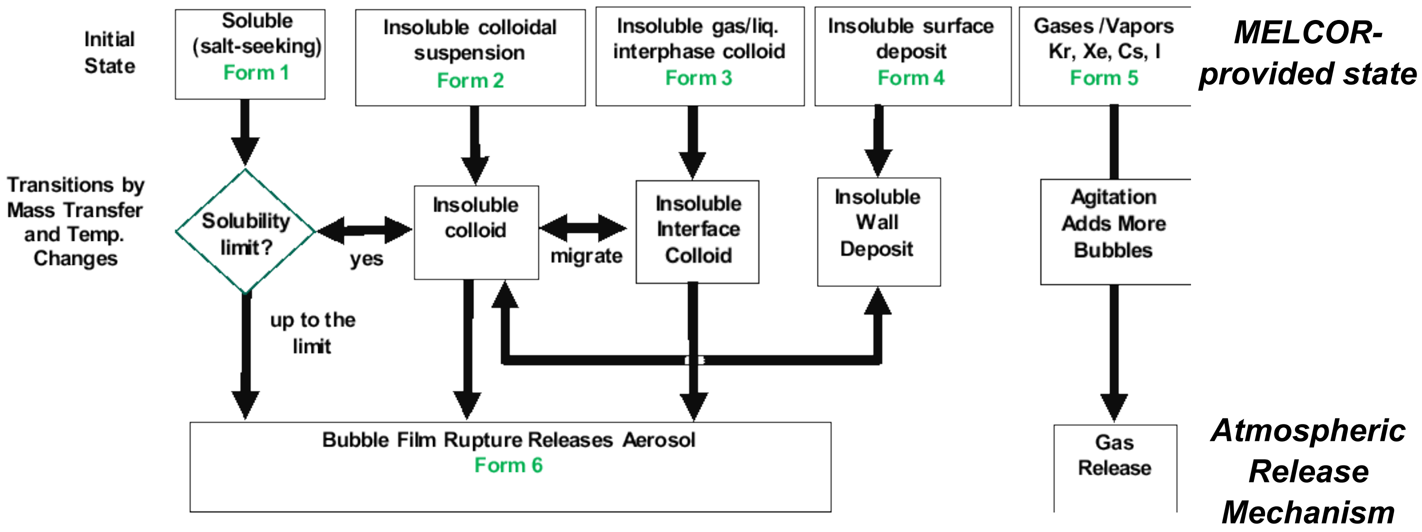
Model Scope

Evaluation of thermochemical state
- Gibbs Energy Minimization with Thermochimica
- Provides solubilities and vapor pressures

Thermodynamic database
- Generalized approach to utilize any thermodynamic database
- MSTDB has two systems
- Pu-U-Th-Nd-Ce-La-Cs-Rb-Ca-K-Na-F-Be-Li and Pu-U-Cs-K-Cl-Mg-Na-Li

Collaboration underway to inform database developers on severe accident needs
- Iodine, strontium, tritium etc.
- Chemicals introduced in severe accidents such as oxygen and water vapor
- Temperatures much higher than operating temperature

Radionuclides grouped into 6 forms as found in the Molten Salt Reactor Experiment at ORNL



Initial Model Form

Solubility determined from empirical evidence (P. Britt, ORNL 2017)

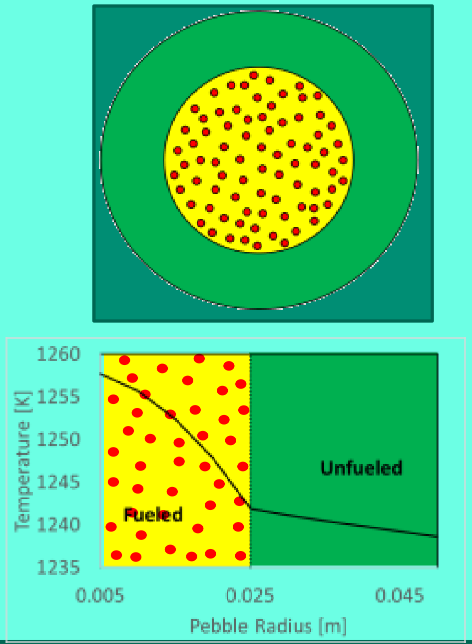
Solubilities mapped to 17 MELCOR fission product classes

Insoluble MELCOR classes are assigned to be colloidal

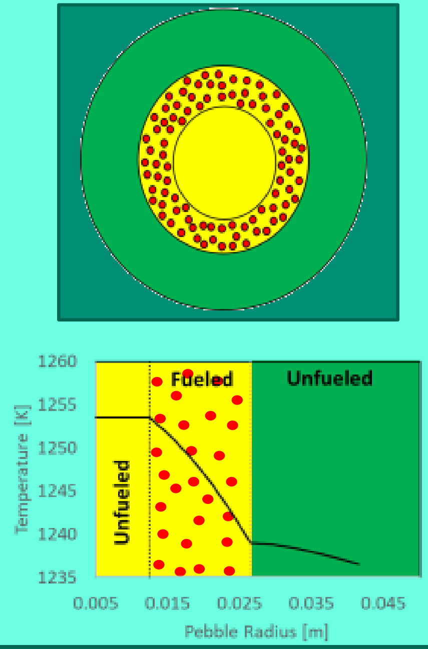
TRISO-related Components

- Pebble Bed Reactor Fuel/Matrix Components
  - Fueled part of pebble
  - Unfueled shell (matrix) is modeled as separate component
  - Fuel radial temperature profile for sphere

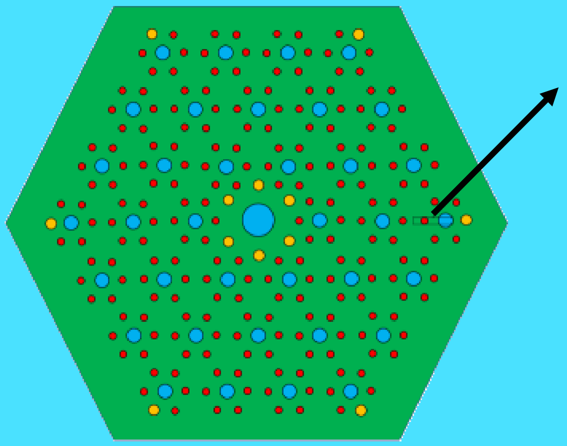
Fueled pebble core

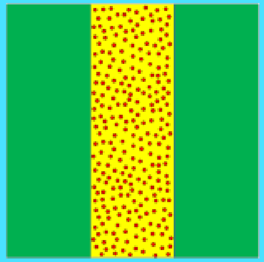


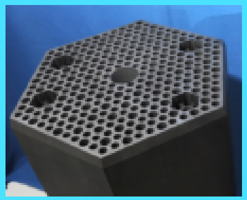
Unfueled pebble core

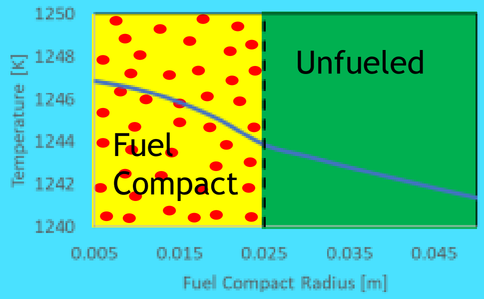


- Prismatic Modular Reactor Fuel/Matrix Components
  - “Rod-like” geometry
  - Part of hex block associated with a fuel channel is matrix component
  - Fuel radial temperature profile for cylinder

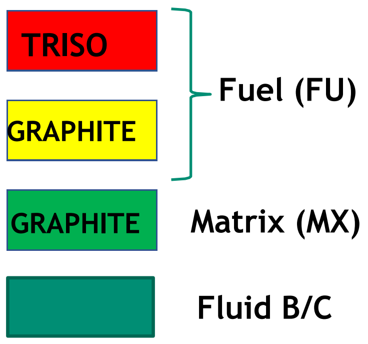


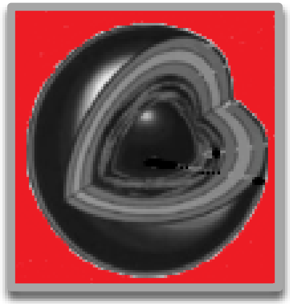






Legend



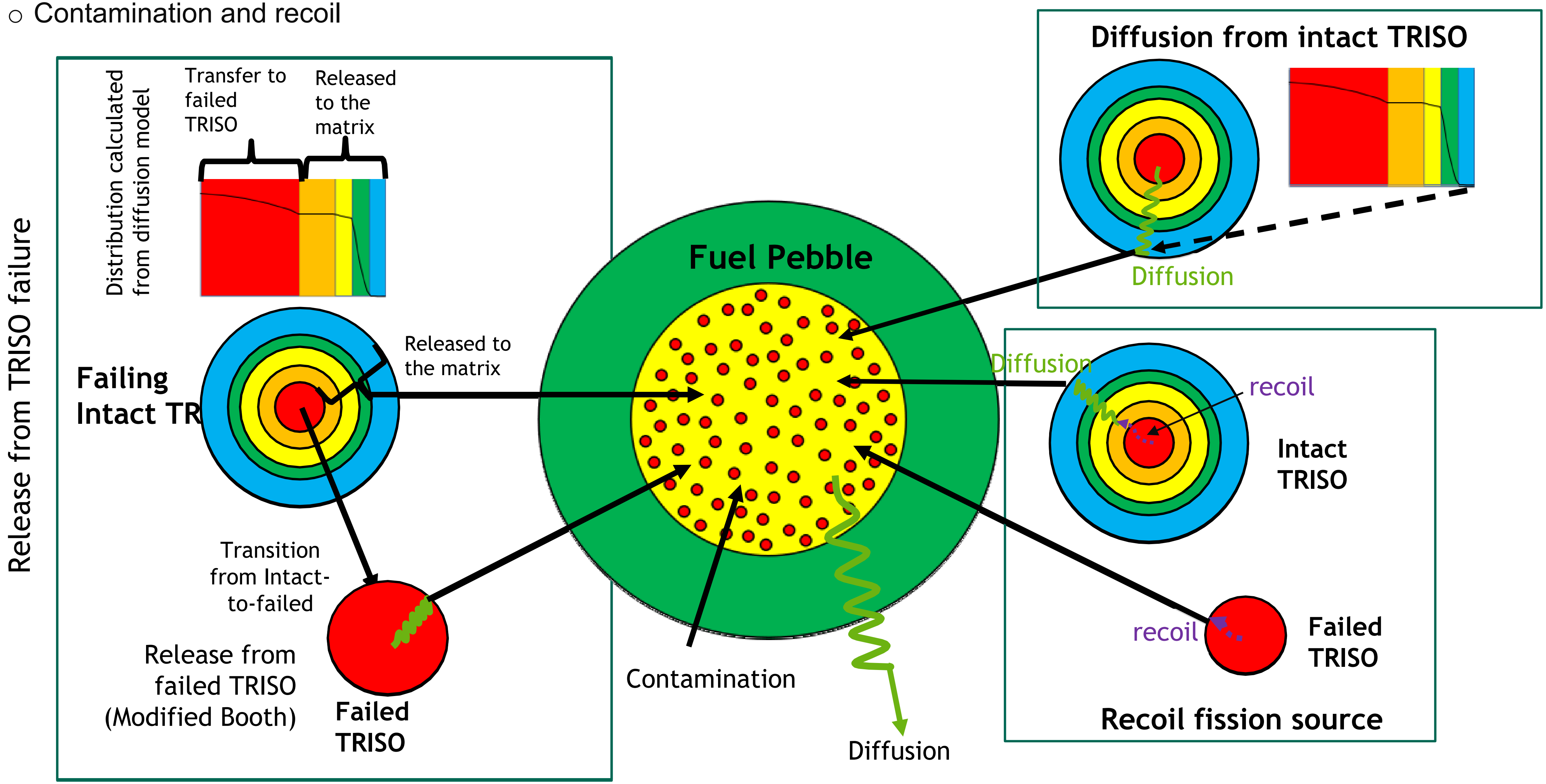


TRISO (FU)

Sub-component model for zonal diffusion of radionuclides through TRISO particle

TRISO Radionuclide Release Models

- Recent failures – particles failing within latest time-step (burst release, diffusion release in time-step)
- Previous failures – particles failing on a previous time-step (time history of diffusion release)
- Contamination and recoil

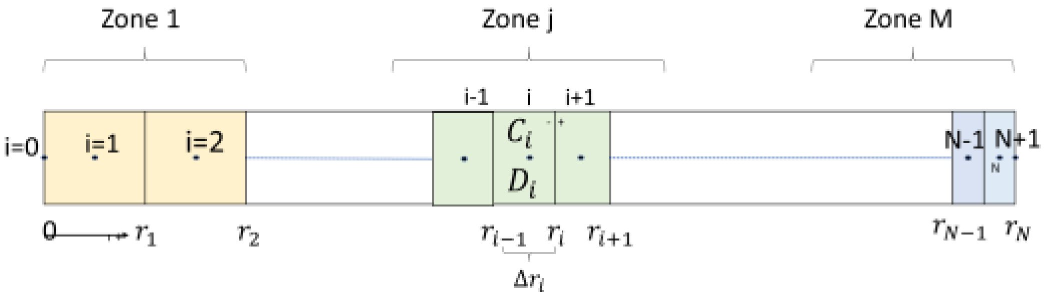


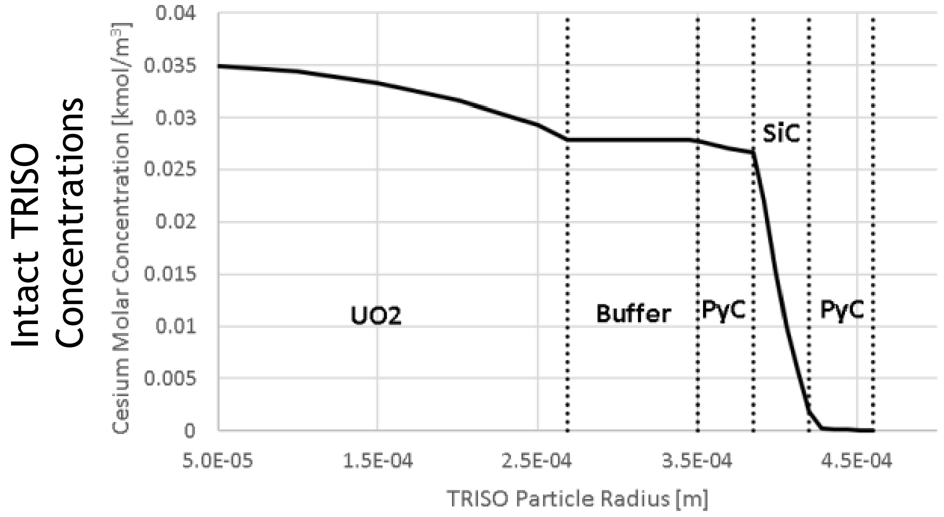
TRISO Radionuclide Diffusion Release Model

Intact TRISO Particles

- One-dimensional finite volume diffusion equation solver for multiple zones (materials)
- Temperature-dependent diffusion coefficients (Arrhenius form)

$$\frac{\partial C}{\partial t} = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n D \frac{\partial C}{\partial r}\right) - \lambda C + \beta \qquad D(T) = D_0 e^{-\frac{Q}{RT}}$$





Diffusivity Data Availability

Radionuclide	UO_2	UCO	PyC	Porous Carbon	SiC	Matrix Graphite	TRISO Overall
Ag	Some	Not investigated	Some	Not found	Extensive	Some	Extensive
Cs	Some		Some		Extensive	Some	Some
I	Some		Some		Some	Not found	Not found
Kr	Some		Some		Not found	Some	Some
Sr	Some		Some		Extensive	Some	Some
Xe	Some		Some		Some	Some	Not found

Data used in the demo calculation

[IAEA TECDOC-0978]

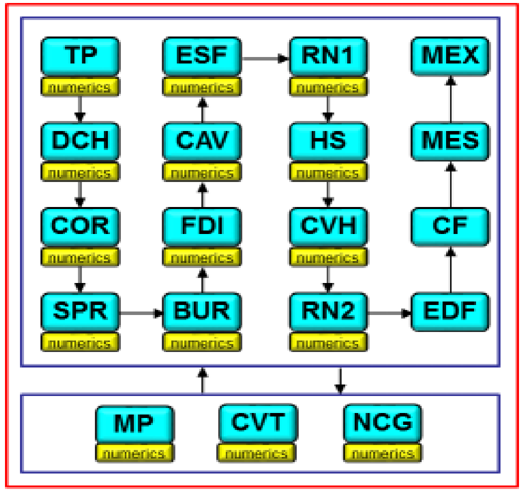
Layer	FP Species							
	Kr		Cs		Sr		Ag	
	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m^2/s)	Q (J/mole)	D (m2/s)	Q (J/mole)
Kernel (normal)	1.3E-12	126000.0	5.6-8	209000.0	2.2E-3	488000.0	6.75E-9	165000.0
Buffer	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0	1.0E-8	0.0
PyC	2.9E-8	291000.0	6.3E-8	222000.0	2.3E-6	197000.0	5.3E-9	154000.0
SiC	3.7E+1	657000.0	7.2E-14	125000.0	1.25E-9	205000.0	3.6E-9	215000.0
Matrix Carbon	6.0E-6	0.0	3.6E-4	189000.0	1.0E-2	303000.0	1.6E00	258000.0
Str. Carbon	6.0E-6	0.0	1.7E-6	149000.0	1.7E-2	268000.0	1.6E00	258000.0

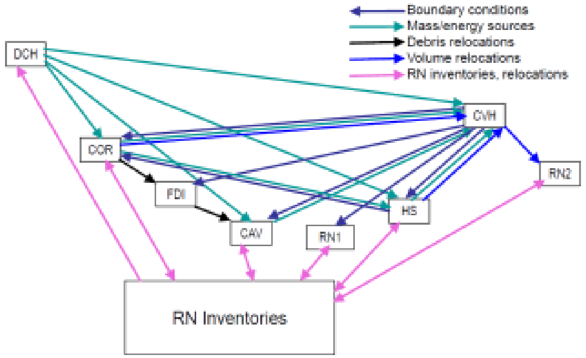
Iodine assumed to behave like Kr

CORSOR-Booth LWR scaling used to estimate other radionuclides

MELCOR Code Architecture Evolution

- Generalized numerical solution engine
- Hydrodynamics
- In-vessel damage progression
- Ex-vessel damage progression
- Fission product release and transport





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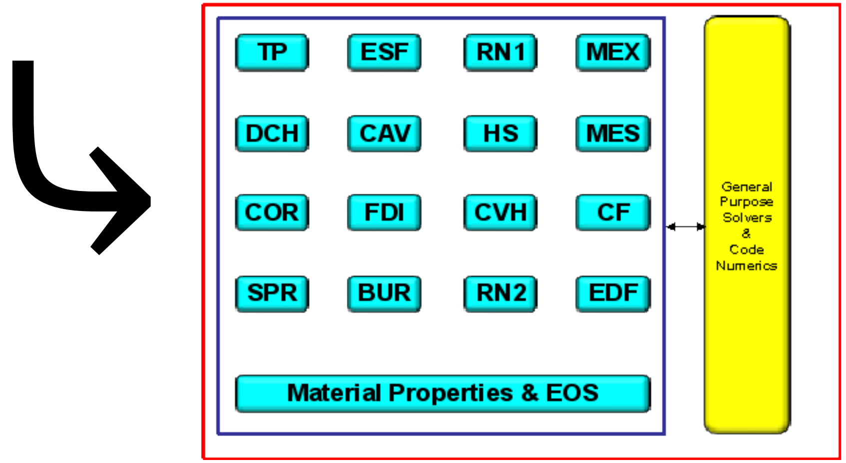
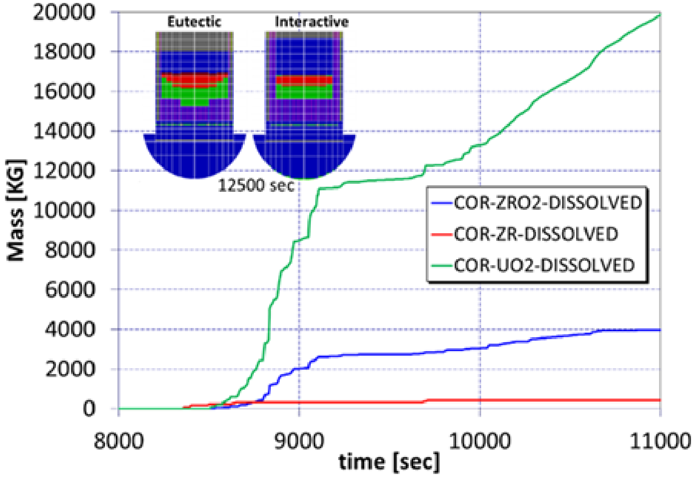
Separate **Physics** & **Numerics**



MELCOR In-Vessel Core Damage Progression

Generalization of the code architecture

- Reduce numerical variability
- Support flexible injection of new physics representations of degradation processes
- Expand scope of uncertainty that can be probed for insights to inform decision -making



Candling model

- MELCOR moves melting material down a component surface (candle) in a single time step
- Such modeling limits oxidation and heat transfer for material in motion

Material interactions

- Enhancements to enable code to more flexibly represent new material systems
- Critical in evaluation of high-temperature material response for range of advanced nuclear energy technologies
- Support generalized treatment of fission product speciation in novel systems
- Rationalize material system with ex-vessel (CAV) package

Lower head structure

- The lower head model to be rewritten to improve the numerical solution of the equations to better account for melting at the interior boundary

COR component objects and restructuring of COR database

- Allow templated creation of component objects
- Carry-over properties such as oxidation, hold-up, number of surfaces in contact with CVH, etc. for new components
- Enhance user flexibility to define COR component attributes for specific design needs