Multiphysics Simulations of Molten Salt Reactors

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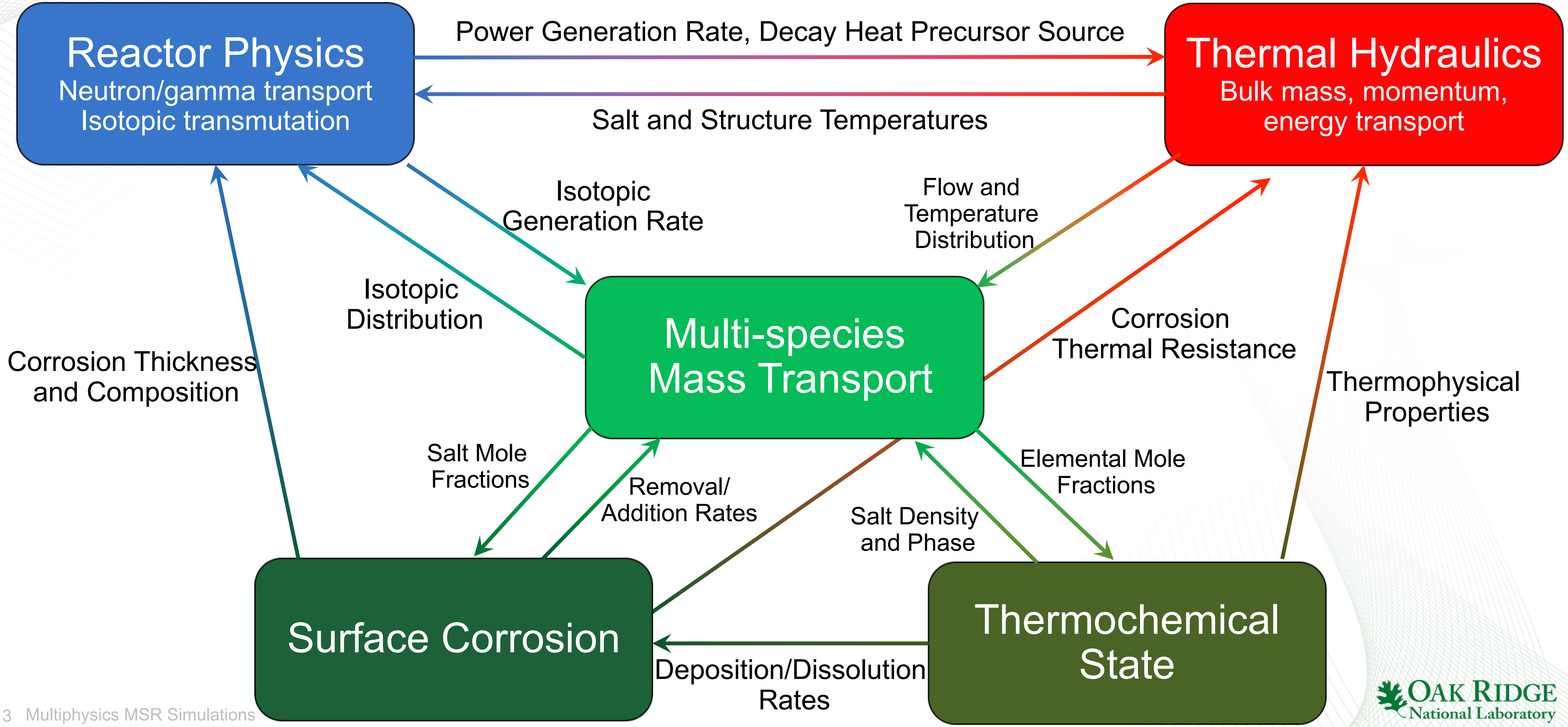
What do we need to model a Molten Salt Reactor?

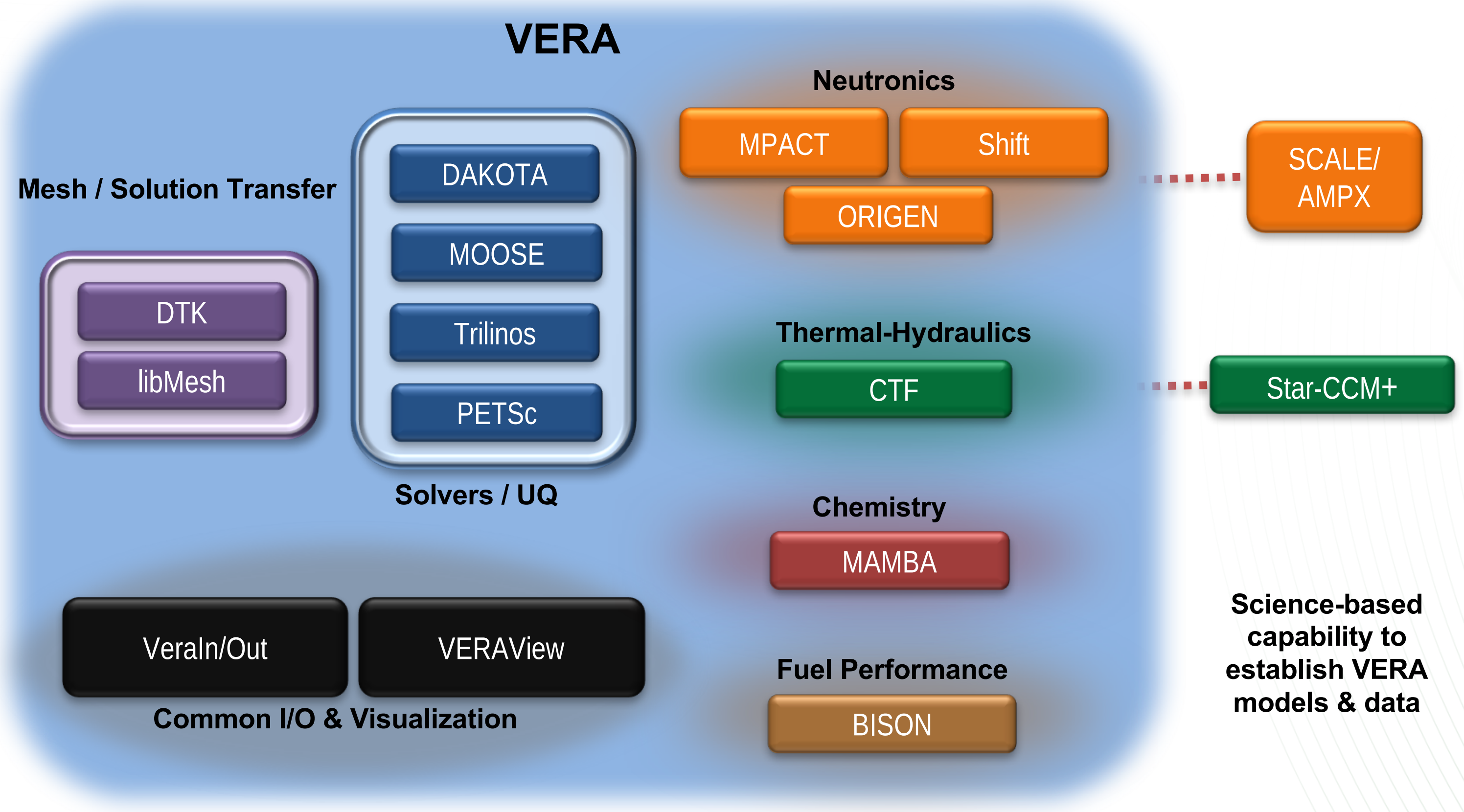
- Reactor Physics
  - Neutron transport, delayed neutron precursor drift, isotopic transmutation
- Thermal Hydraulics
  - Flow and heat transport through upper/lower plenum, core, primary loop
- Thermochemistry
  - Chemical state at a range of temperatures and fission product concentrations
- Mass Transport
  - How are species moving through the solution
- Corrosion
  - How much and where

Multiphysics simulations are required for MSRs



Adapting CASL tools for MSR analysis

- In FY17, ORNL funded an LDRD to adapt tools developed for the CASL program to model molten salt reactors



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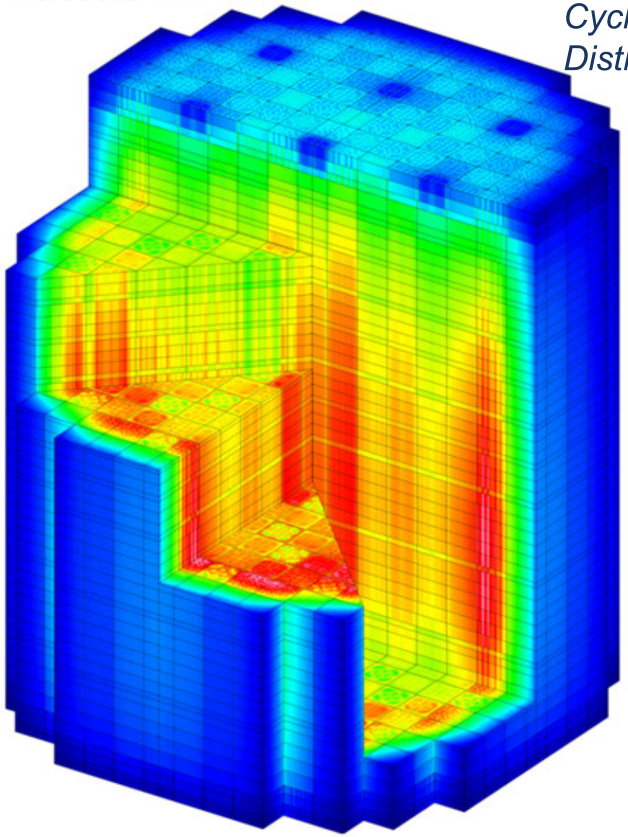
VERA Core Simulator Methods

Virtual Environment for Reactor Applications

WB1C11 Beginning-of-Cycle Pin Power Distribution

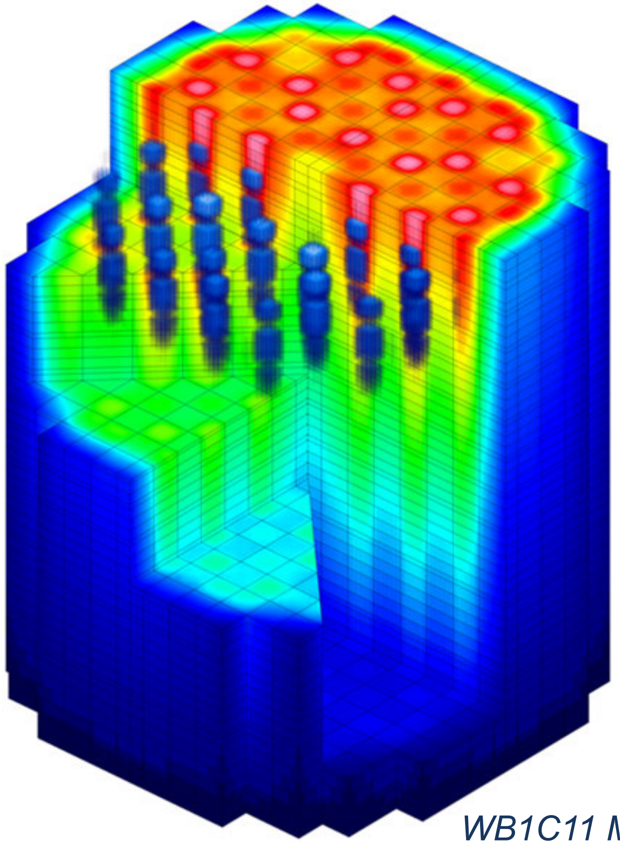


MPACT

Advanced pin-resolved 3-D whole-core neutron transport in 51 energy groups and >5M unique cross section regions

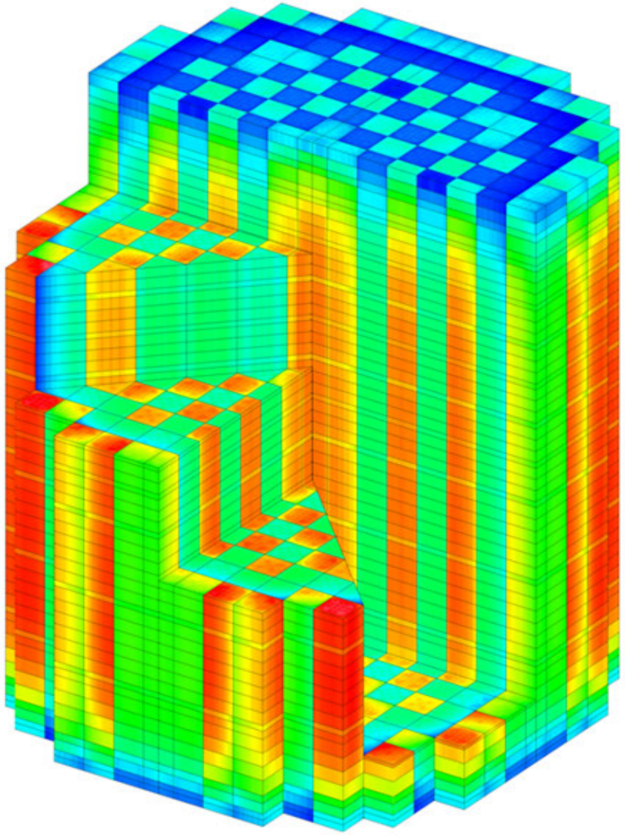
CTF

Subchannel thermal-hydraulics with transient two-fluid, three-field (i.e., liquid film, liquid drops, and vapor) solutions in 14,000 coolant channels with crossflow



WB1C11 Middle-of-Cycle Coolant Density Distribution

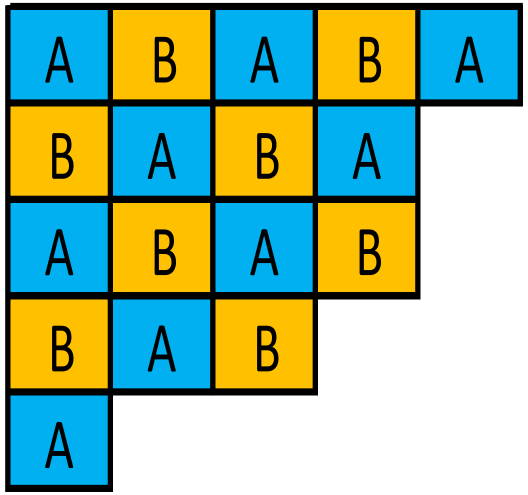
WB1C11 End-of-Cycle Pin Exposure Distribution



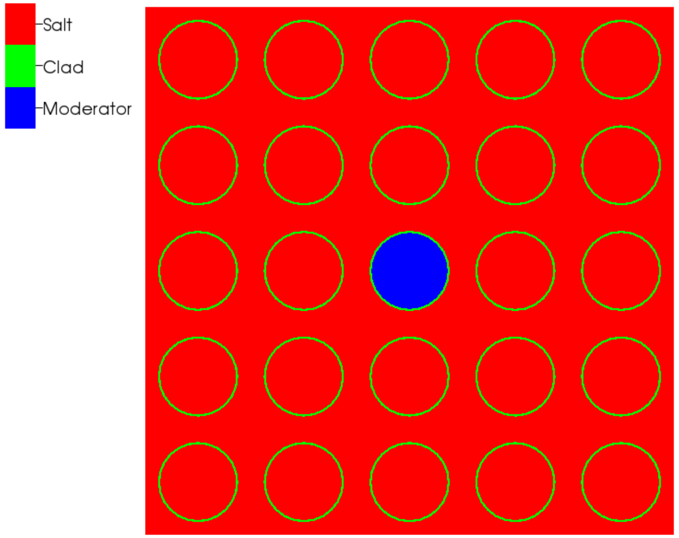
ORIGEN

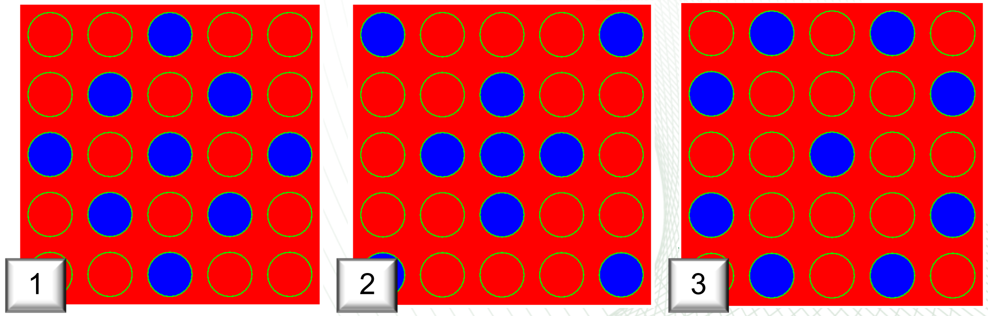
Isotopic depletion and decay in >2M regions tracking 263 isotopes

Initial simulations of TransAtomic-like Design



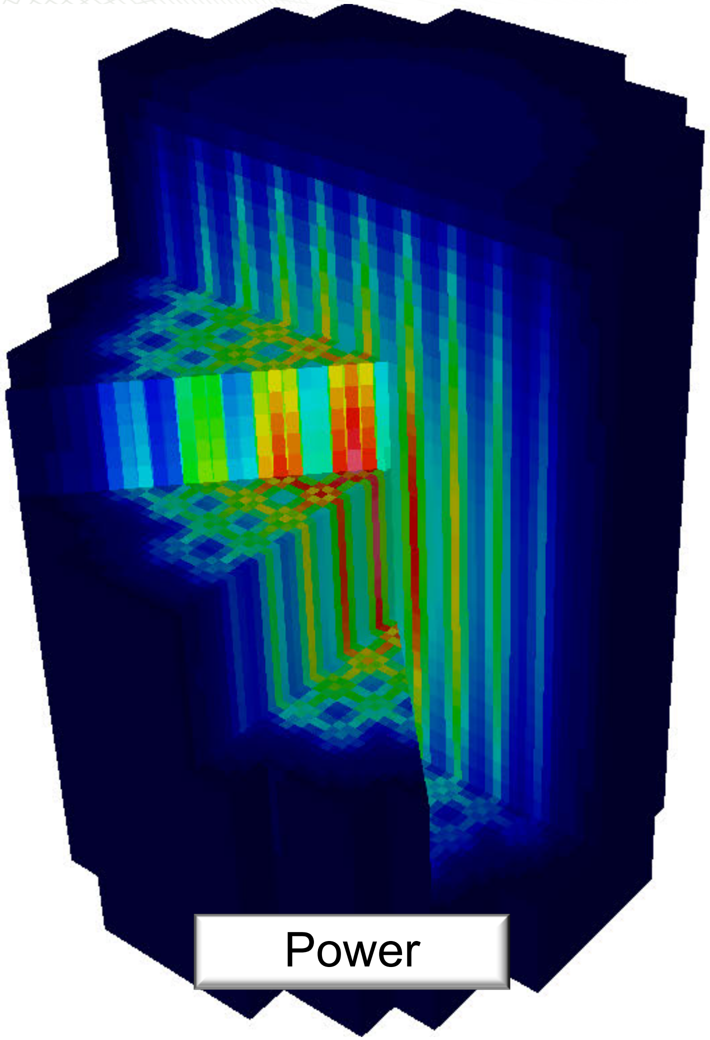
- Models for MPACT and CTF are built based on updated geometry specifications (5x5 rod arrays / 68 assemblies)
  - Zirconium hydride rods inserted into uranium fluoride salt
  - Moderator rod banking strategy approximated similar to LWRs
  - Assumed guide tubes around moderator rod locations

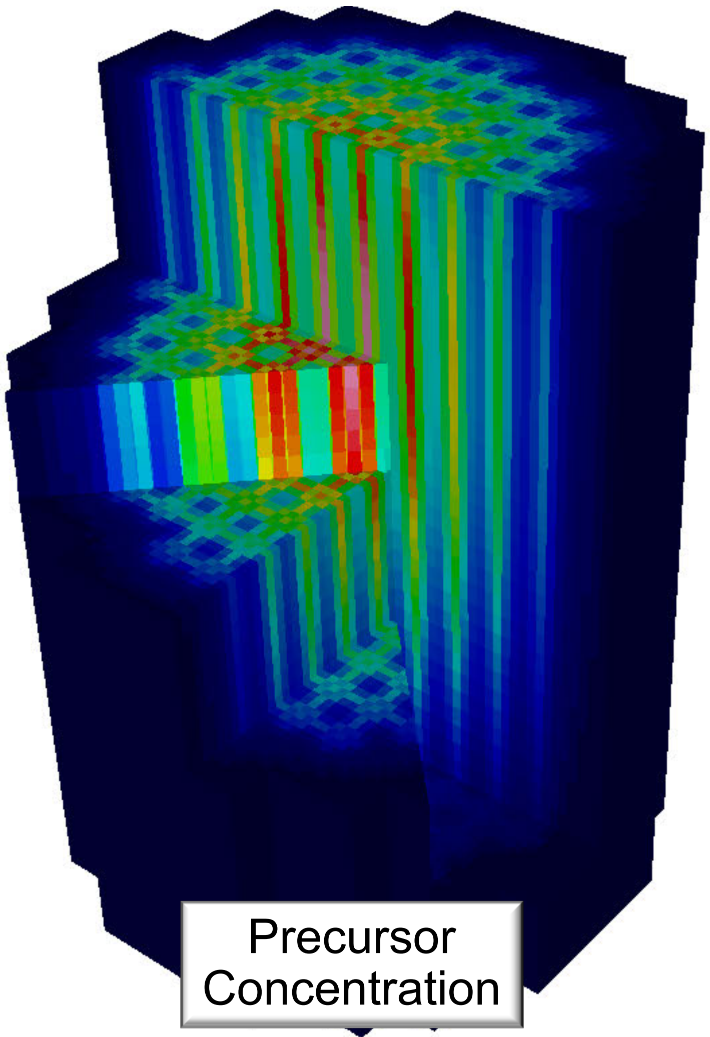


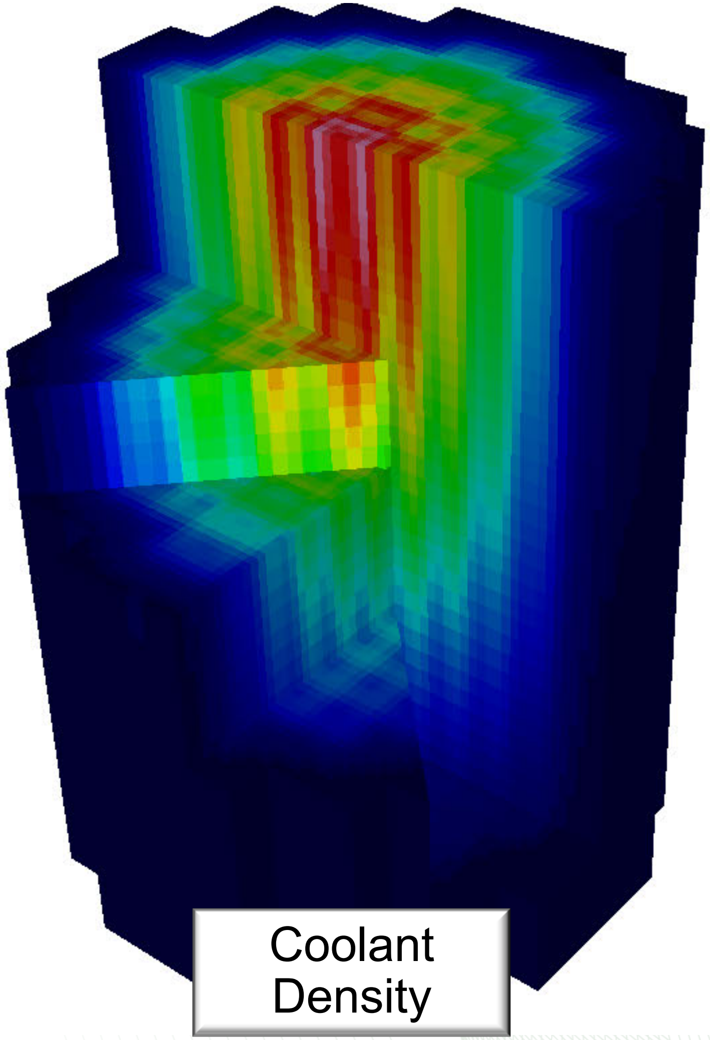


"Transatomic Technical White Paper, V 2.0," http://www.transatomicpower.com, Transatomic Power Corporation (July 2016), Accessed July 2016.

Initial critical configuration based on rod search



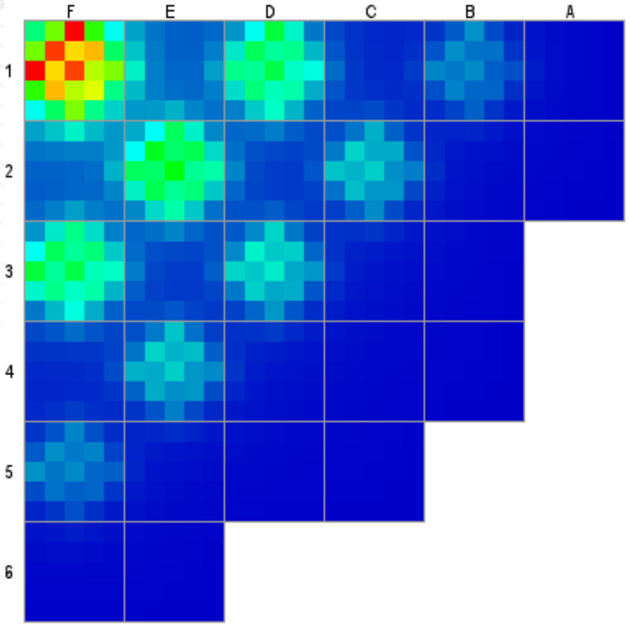




Critical configuration

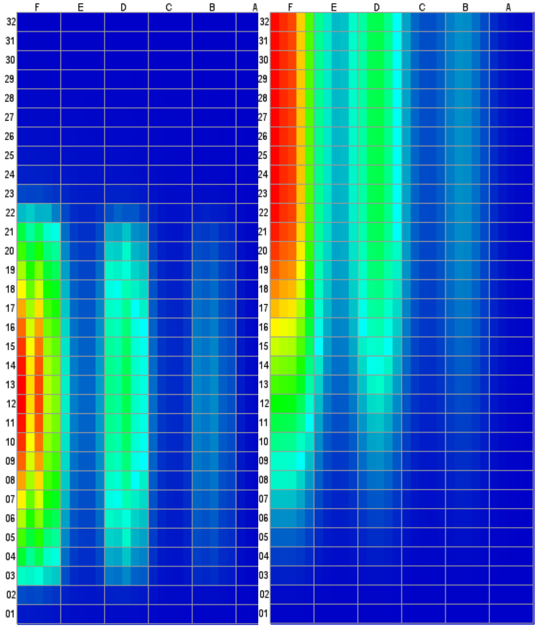
First moderator bank inserted to 66%

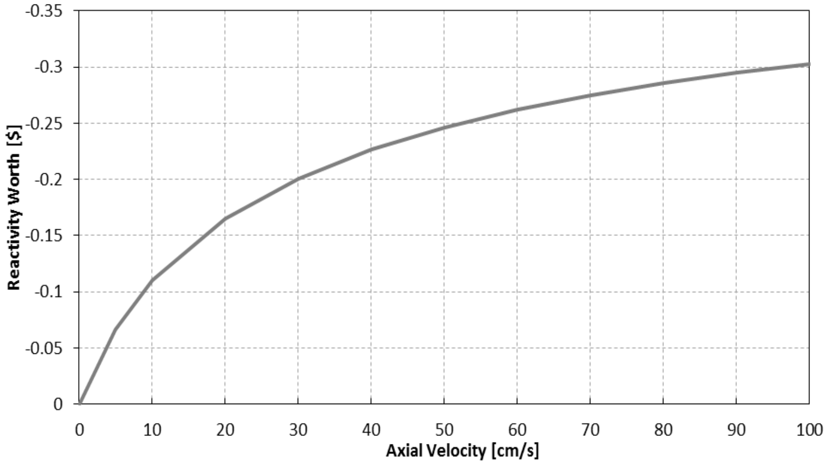
Radial Power Distribution



Axial Power Distribution

Axial Temp Distribution

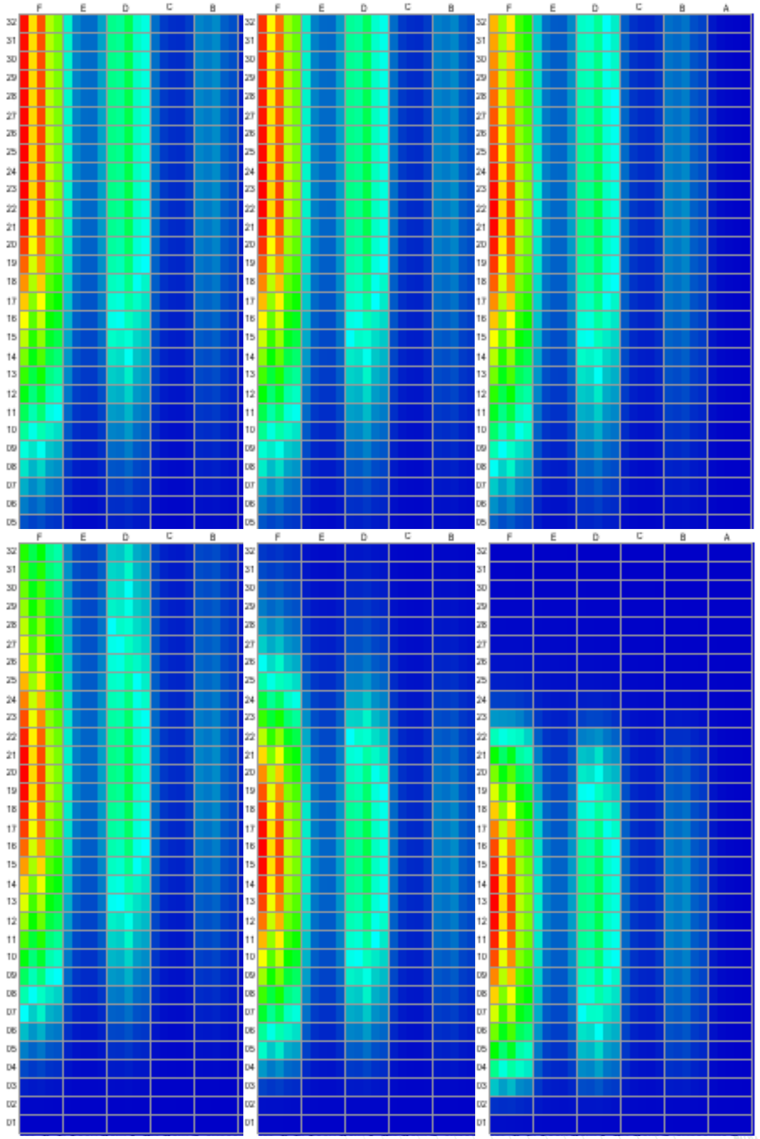




Group 1 T=55.45 s

Group 2 T=21.80 s

Group 3 T=6.36 s



Group 4 T=2.19 s

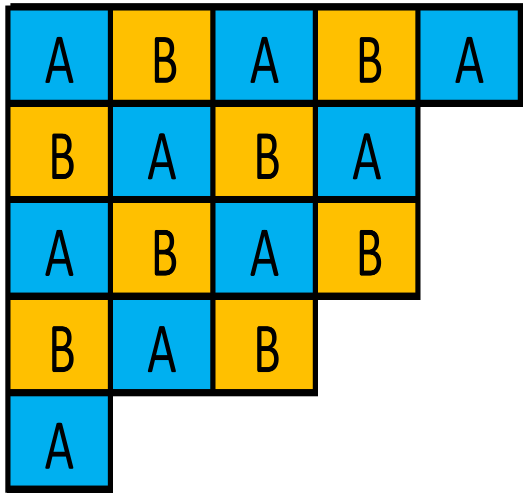
Group 5 T=0.51 s

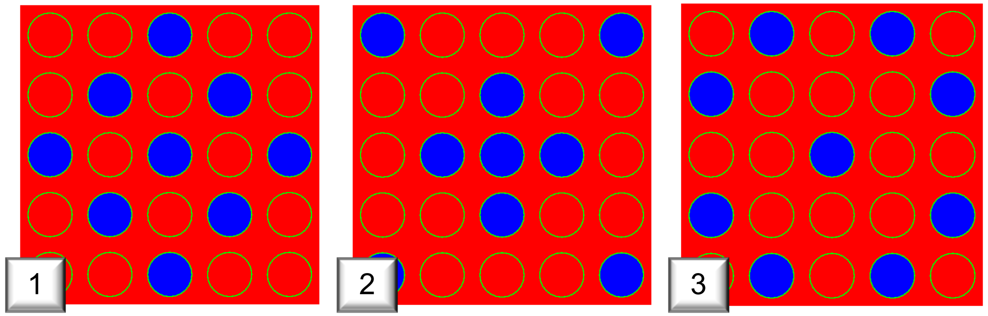
Group 6 T=0.08 s

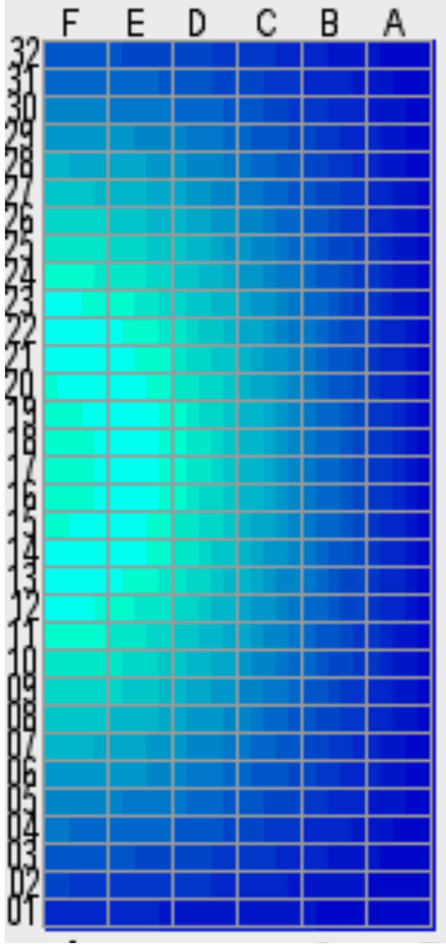
Delayed Neutron Precursor Concentrations

Core depletion with moderator rod insertion

- Moderator rod insertion occurs in banked strategy
  - A-1, B-1, A-2, B-2, etc.
- Reactor is depleted at nominal power and bank position is determined by criticality search







Power Shape Evolution with Moderator Rod Inserted

Mass Transport Modeling and Simulation Progress

- **Based on ongoing review of the MSRE documentation**

Mechanistic Theory

- Development of multicomponent, thermo-chemical governing equations of transport for mixtures of salts undergoing fission
- Coupled redox chemical reactions and nuclear reactions
- Rigorous ionic diffusion via chemical activity

Modeling

- Volume-averaged two-phase, multicomponent fluid mixture
- Focus on volatile fission products (*e.g.* Xe)
- Channel flow average model for MSRE geometry for implementation in CTF
- Leverage thermochemistry

Simulation

- Extend CTF code to thermo-chemical transport
- Coupling to ORIGEN for source terms of fission products
- Coupling to thermochemistry through Thermochemica

Mass Transport with Nuclear Decay

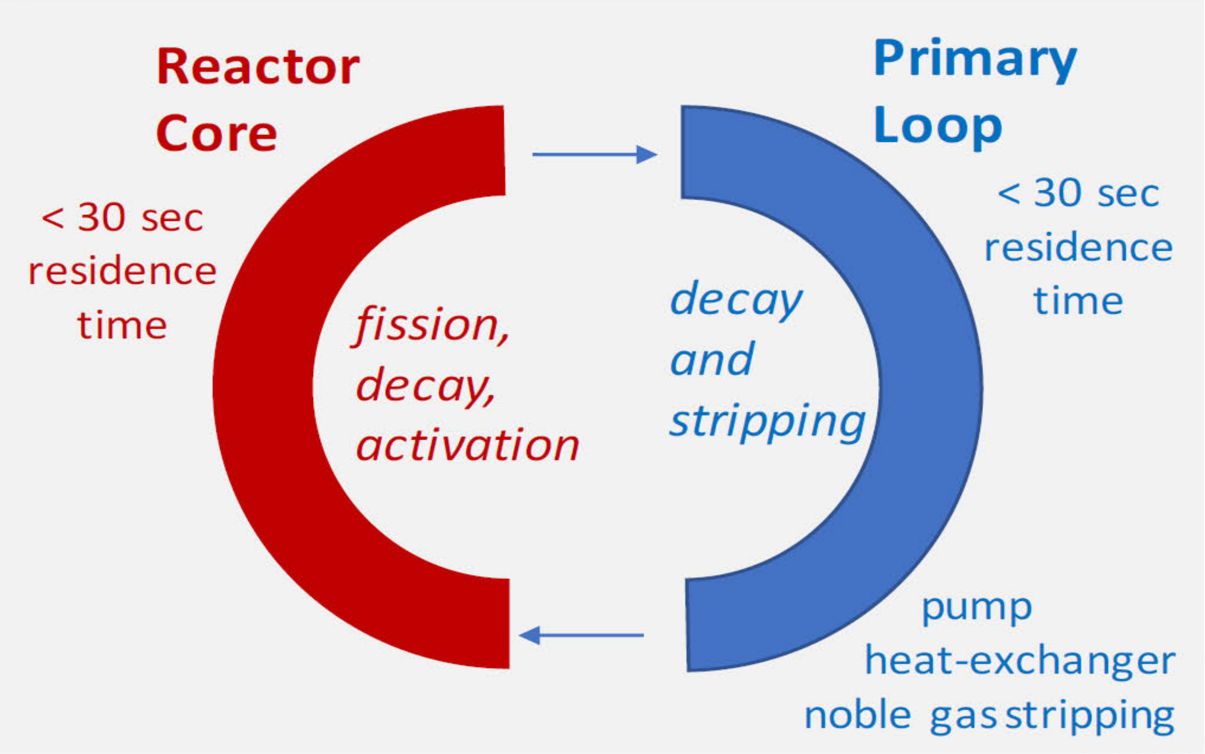
$^{137}I \longrightarrow {}^{137}Xe \longrightarrow {}^{137}Cs$

25 sec. 4 min.

$^{99}Zr \longrightarrow {}^{99}Nb \longrightarrow {}^{99}Mo \longrightarrow {}^{99}Tc$

2.1 sec. 15 sec. 2.75 days

soluble
sometimes soluble
insoluble
gaseous



$^{131,132}Cd \longrightarrow {}^{131}In \longrightarrow {}^{131}Sn \longrightarrow {}^{131}Sb \longrightarrow {}^{131}Te \longrightarrow {}^{131}I \longrightarrow {}^{131}Xe$

<1 sec <1 sec 1 min. 23 min. 25 min. 8 days

Mixture Theory for Molten Salts in Fission

- **Single-phase development in progress**

  - **Multicomponent balance of mass**

mixture mass-average velocity

mass-average diffusion flux

# of species

$$\partial_t \rho_a + \mathrm{div}_{\boldsymbol{x}}(\rho_a \boldsymbol{v}) = -\mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{j}_a + r_a \quad a = 1, \ldots, N$$

reaction source

→ constitutive equation function of chemical potentials, temperature, and pressure

→ chemical reaction mechanisms, kinetics models, decay

  - **significant undertaking; progressive development**

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Mixture Theory for Molten Salts in Fission (cont.)

- **Mixture balance of momentum**

mixture mass density

mixture stress tensor

$$\partial_t(\rho \boldsymbol{v}) + \mathrm{div}_{\boldsymbol{x}}(\rho\, \boldsymbol{v} \otimes \boldsymbol{v}) = \mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{T} + \rho\, \boldsymbol{b}$$

mixture body force

$$\boldsymbol{T} := \sum_a \boldsymbol{T}_a - \sum_a \rho_a^{-1}\, \boldsymbol{j}_a \otimes \boldsymbol{j}_a,$$

species stress

stress-diffusion coupling

- **unknown territory; starting with simple assumptions**

Mixture Theory for Molten Salts in Fission (cont.)

- **Mixture balance of energy (single temperature)**
- **Mixture imbalance of entropy**

- This is work in progress to state consistent energy balance and entropy considerations for the development of constitutive equations
- A turbulent model may be needed sooner than later
- A gas-liquid interface mass transfer model will be next in development focused on volatile fission products

Conclusions and Future Work

- Molten Salt Reactors require multiphysics simulations to understand the behavior of the salt and reactor components throughout the lifetime of the reactor
- Initial conversion of CASL tools focused on traditional core simulator and the development of a new mass transport component
- Continuing work in FY18 will focus on
  - Integration of thermochemistry and surface corrosion models
  - Extension of core simulator for other reactor designs
  - Validation of coupled system against existing MSRE data

Questions

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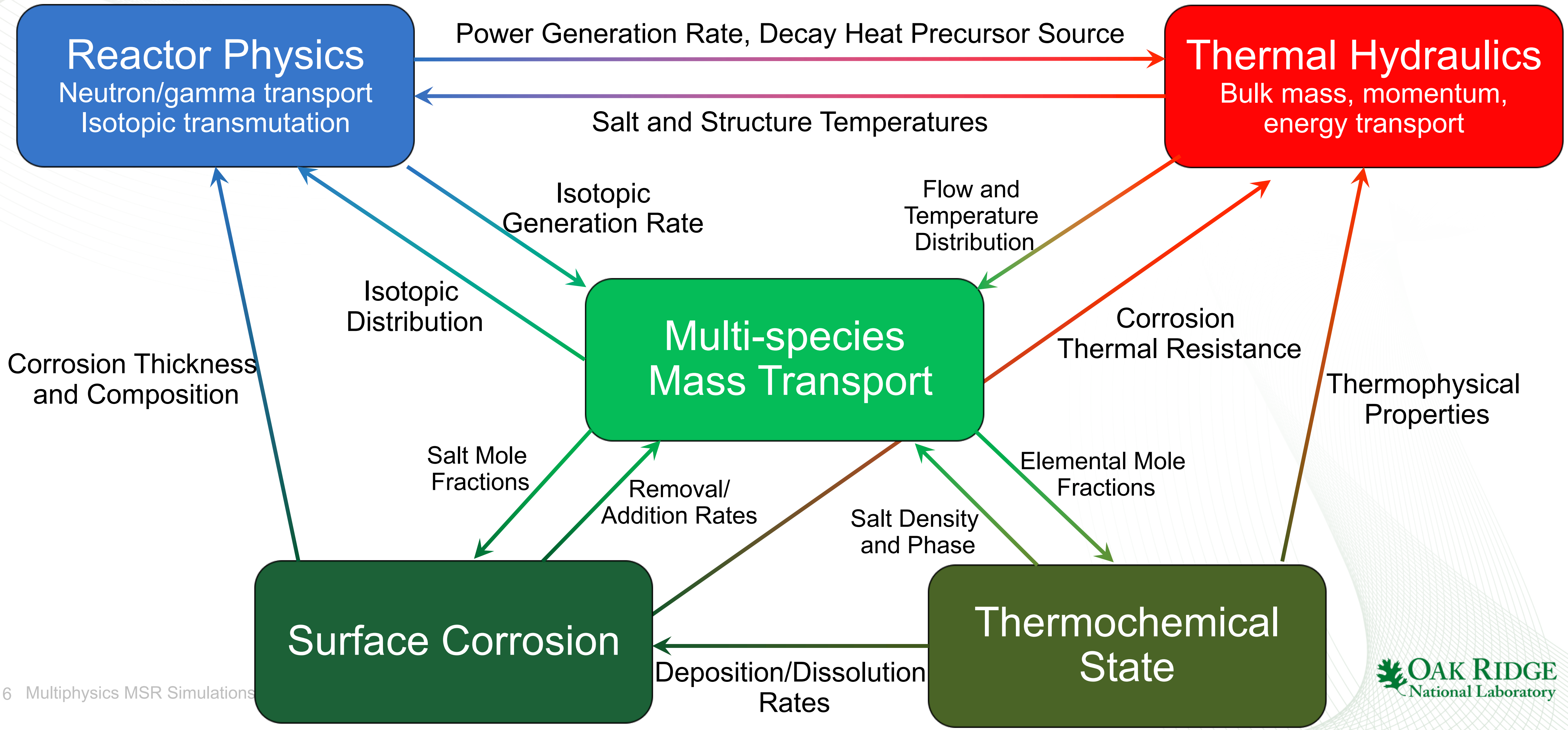

Noble Metals Mass Transport

- **Rigorous continuum theory, modeling, and simulation needed for noble metals**

ORNL/TM-1972/3884

Table 5.1

Noble Metal Distribution in the MSRE*

	During ^{235}U Runs	During ^{233}U Runs
Noble Metals on Heat Exchanger Surfaces	40%	6%
Noble Metals on Other Hastelloy-N Surfaces in Fuel Loop	50	8
Noble Metals on Graphite Surfaces in Core	1	0.4
Noble Metals in Pump Bowl, Overflow Tank, Off-Gas System, etc. (by Difference)	9	86
	100%	100%

- Dispersion of species in the system is a reflection of complex thermo-chemical transport
- Noble metals fate was controversial in the MSRE
- Reactor operation changes were not correlated with findings

- **Fission reactions may substantially affect mass transport in molten salts**
- **We are addressing this overlooked underlying phenomena**