Molten Salt Reactor
PROGRAM

MSR Source Term Development for the MELCOR Severe Accident Code

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SAND2026-19991C

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MELCOR for Advanced Nuclear Energy Technologies

Fully integrated, engineering-level code

- Thermal-hydraulic response of reactor coolant system, reactor cavity, rector enclosures, and auxiliary buildings
- Core heat-up, degradation and relocation
- Core-concrete interaction
- Flammable gas production, transport and combustion
- Fission product release and transport behavior

Level of physics modeling consistent with

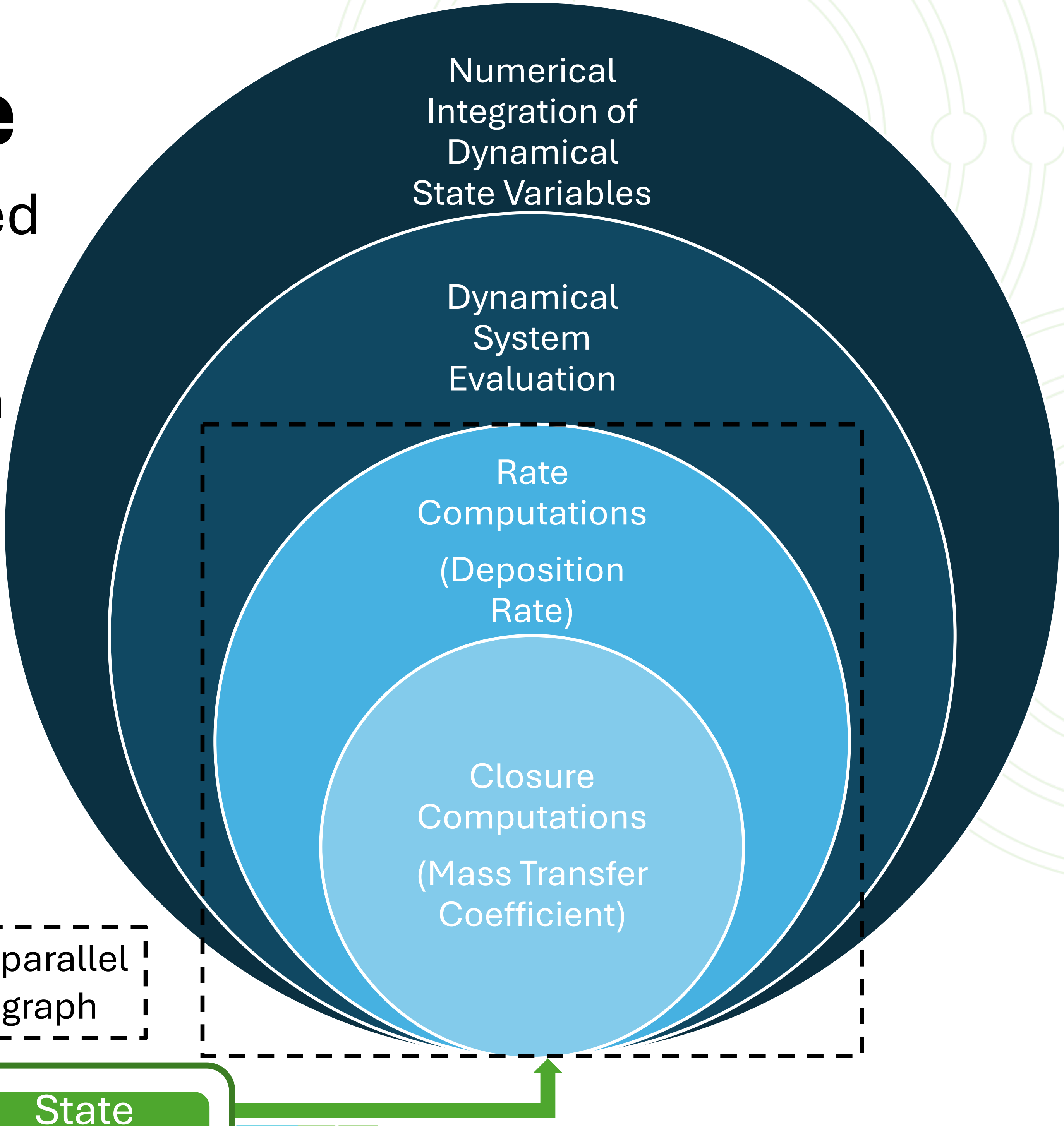
- State-of-knowledge
- Necessity to capture global plant response
- Reduced-order and correlation-based modeling

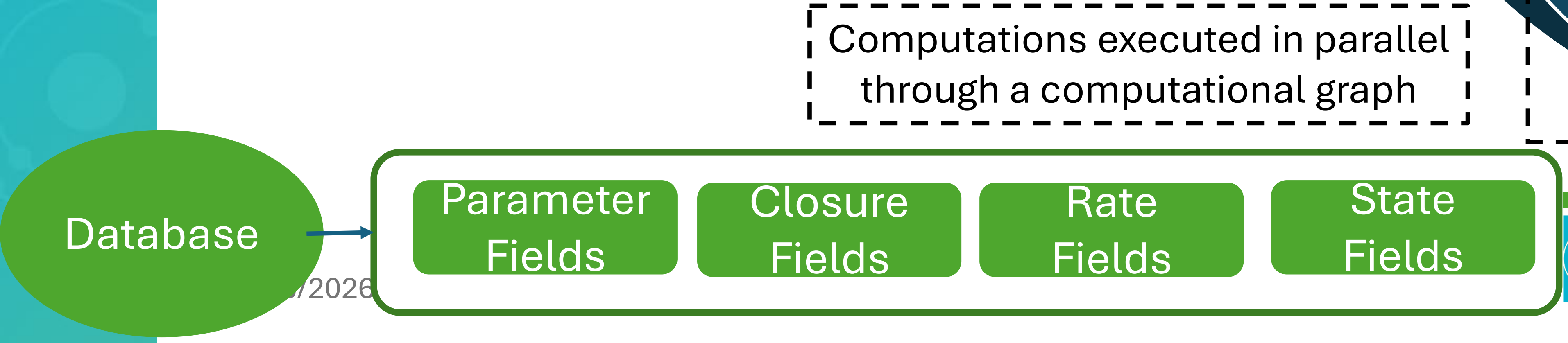
Traditional application

- Models constructed by user from basic components (control volumes, flow paths and heat structures)
- Demonstrated adaptability to range of reactor designs – LWR, LWR-SMR, FHR, HPR, HTGR, MSR, SFR, ATR, VVER, SFP...

Generalized Architecture

- MELCOR modernization has established a new software platform
- Rapid capability implementation through physics/chemistry generalizations
- Generalized means re-using physics equations but changing system state variables
- Numerics **separated** from physics



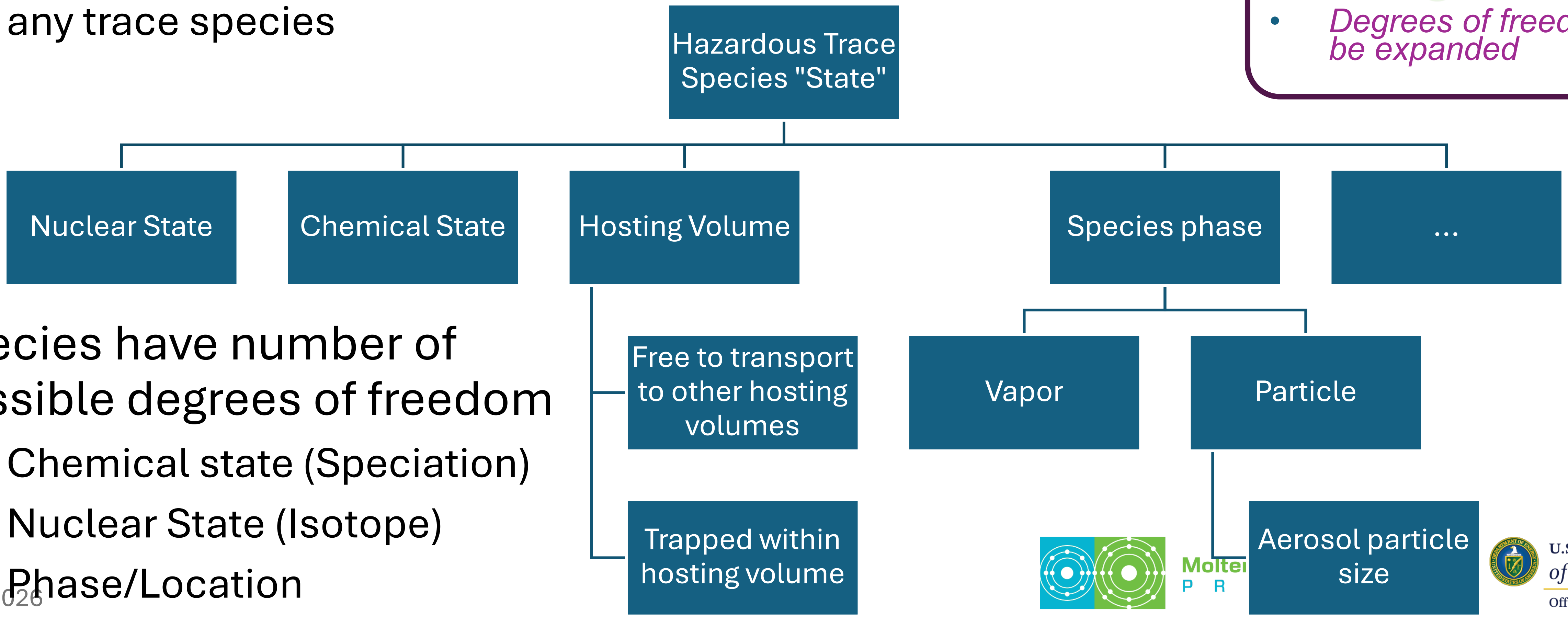


RN Package Generalized Representation of Degrees of Freedom

- Generalize RN package for species transport modeling
  - RN package initially intended to model radionuclide transport
  - Has evolved with MELCOR to generally characterize transport of any trace species

Generalized mathematical representation in software

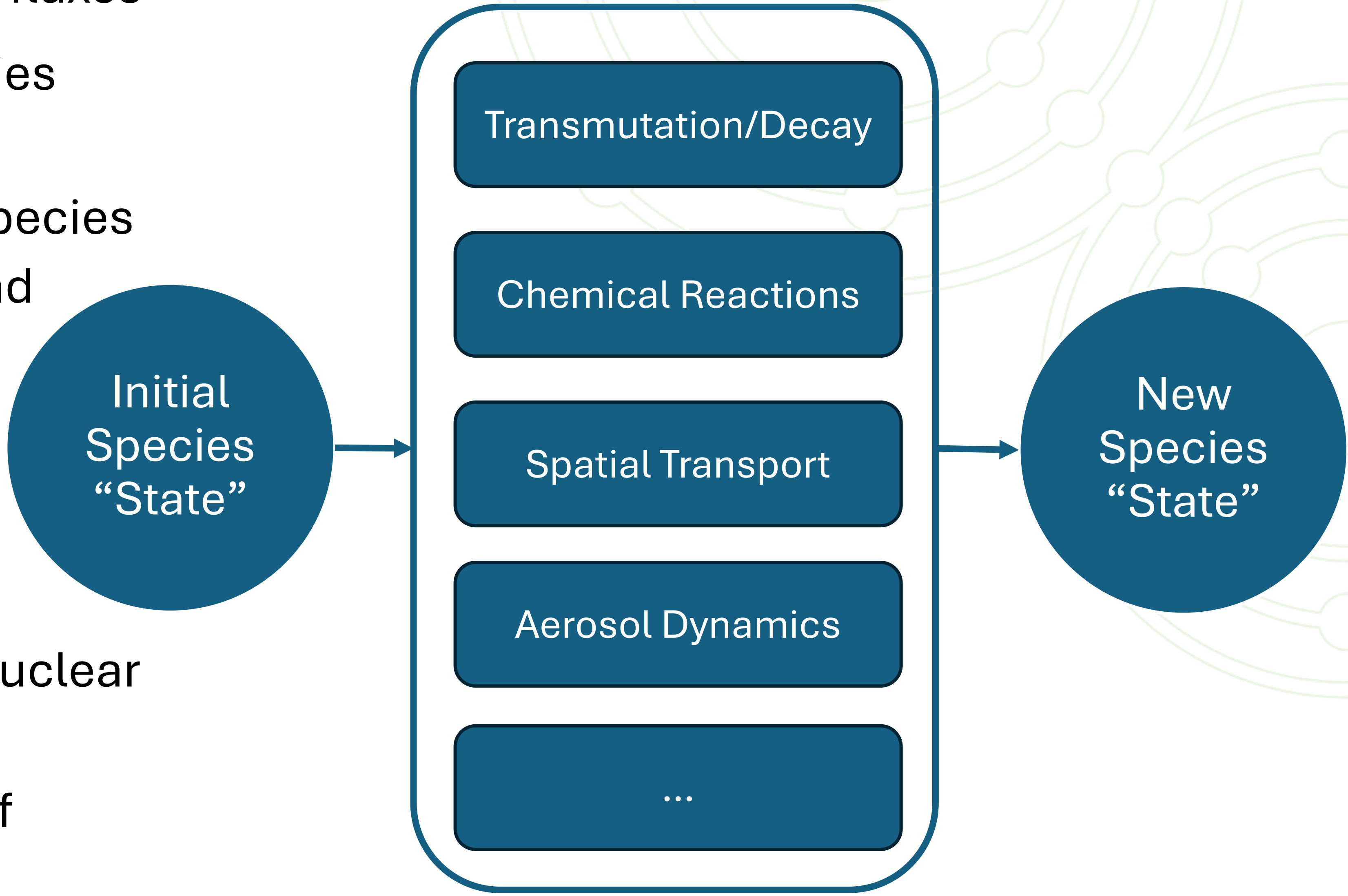
- *Degrees of freedom designed to be expanded*



- Species have number of possible degrees of freedom
  - Chemical state (Speciation)
  - Nuclear State (Isotope)
  - Phase/Location

RN Package Generalized Dynamics

- Species transport is formulated as mass fluxes
- **Interfacial Transport:** Transport of species between "volumes"
- **Aerosol Dynamics:** Transformation of species within volumes associated with vapor and aerosol dynamics
- **Nuclear Processing:** Transformation of species within hosting volumes due to nuclear transmutation and decay
- **Chemical Processes:** Transformation of species within hosting volumes due to chemical reactions



Summary of FY25 and FY26 Activities

- FY2025
  - Implemented Dittus-Boelter, thermophoretic and gravitational solid-deposition models into MELCOR, with focus on noble metals (SAND2025-12380)
- FY2026
  - Complete model implementation and demonstration of a particle size distribution model in MELCOR
  - Complete the development, demonstration and validation of noble gas transport in MSRs using MELCOR (Just started)

Motivations: Reactor Surfaces were Primary Sink for Noble Metals

- Noble metal mass accountancy was inconclusive due multiple test contaminations
- Majority of noble-metal is in circulation
- Deposits occur as an accumulation of finely divided well-mixed material
- Colloids can grow on surface, then dislodge and re-enter reactor circulation

Noble metal deposition fractions (observed/theoretical) for different reactor locations
ORNL-4865

Will concentrate on initial metal deposition

Deposition Models Tested

- Dittus-Boelter mass transfer captures turbulent diffusion deposition

$$D = \frac{k_B T_l}{6\pi\mu_l r_p} \longrightarrow Re = \frac{\rho_l U_l L}{\mu_l}, \mathrm{Sc} = \frac{\mu_l}{\rho_l D} \longrightarrow k_{DB} = 0.023\frac{D_p}{L}Re^{0.8}Sc^{0.4} \longrightarrow \frac{\partial C}{\partial t} = \frac{1}{V}k_m A(C_B - C_s)$$

- Talbot approximation captures thermophoretic deposition

$$Kn = \frac{\mu_l}{\rho_l L}\sqrt{\frac{m_p \pi}{2k_B T_l}} \longrightarrow k_T = \frac{2\mu_l(\frac{k_l}{k_p} + Kn)}{L\rho_l(1+2Kn)(1+2\frac{k_l}{k_p} + 2Kn)}\frac{\nabla T}{T_l} \longrightarrow \frac{\partial C}{\partial t} = \frac{1}{V}k_T A C_B$$

- Richardson-Zaki captures gravitational deposition

$$v_s = \frac{d_p^2(\rho_l - \rho_l)g}{18\mu_l} \longrightarrow \frac{\partial C}{\partial t} = \frac{1}{V}v_s A C_B$$

Mass Transfer Coefficient Dependence on Salt Properties

Kedl parameters

- Purple dots are Kedl's Dittus-Boelter fixed mass transfer coefficients
- Higher diffusion coefficient increases Dittus-Boelter mass transfer coefficient
- Thermophoretic transport will dominate in salts with high viscosity

Viscosity effects mass transport more than salt density

Mass Transfer Coefficient Dependence on Particle Properties

- Kedl's fixed diffusion coefficient only matches one reactor section
- Kedl uses larger diffusion coefficient than observed
- Diffusion coefficient will change in different salt compositions (non-transferable)
- Deposition will transition from Dittus-Boelter to gravitational forms as particle size grows

Particle radii drives mass deposition

Impact of Noble Metal Species and Particle Size on Mass Deposition

- Rate calculation includes temperature dependency for salt density and viscosity
- Small differences between elements in a given salt
- Differences between salts don't appear till 20 minutes
- Using particle sizes observed from MSRE instead of atomic radii significantly decreases noble metal deposition
- No element distinction at larger particle sizes

Particle radii will have strong influence on deposition rate

Impact of Salt Flow and Temperature

- Calculations are for 50 Å radius Mo in FLiNak
- Low flow decreases deposition rate by 1.5% after 60 minutes, increases 0.5% with 33% flow increase
- Decreasing temperature by ~50K decreases deposition rate by 0.5%/hr while increasing temperature by 78 K increases deposition by 1%/hr

Influence of salt velocity on deposition needs better understanding

FY25 Summary

- Turbulent, thermophoretic and gravitational deposition models were implemented into MELCOR
- Estimated particle diffusion coefficients through salts are much lower than those previously reported
- Particle size and diffusion, and salt temperature, flow and viscosity were found to be drivers for noble metal deposition
- Deposition rates were found to have no dependence on species at MSRE observed particle sizes
- Dependency on salt flow rate shows importance for carrying out dynamic salt loop tests instead of static testing.

FY25 Results Showed Strong Dependence on Particle Size for Deposition

- Not surprising given deposition equations dependence on particle radius
- The reactor will have a distribution of particle radii at any time
- Distribution will depend on reactor operations and salt operations
- Population balance equations (PBE) describe how number distributions evolves over time and space due to transport and associated processes
- Aerosol models have previously demonstrated accurate models for particle size distribution

Create a solid PBE using a sectional approach like with Aerosols

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Sectional Theory Divides Particle Size into Discrete Bins

- Tracks the particle concentration in each section, preserving resolution across the full distribution
- Converts the continuous population balance equation into a tractable system of couple equations for numerical solution
- Naturally represents key particles processes such as nucleation, aggregation and breakage
- Offers strong balance of accuracy interpretability and computational practicality for engineering transport codes

Particle Sectional Representation

Size-space representation of particle processes

Differences Between Aerosol and Solid Particles

Aerosols in Gas

- Suspended in a gas
- May require slip correction
- Collision efficiency often near 100%
- Growth by condensation/evaporation
- Breakage often negligible

Particles in Liquid

- Suspended in a liquid
- Usually in the continuum regime
- Strongly affected by surface/solvent forces
- Growth by nucleation, growth, dissolution
- Breakage often important

Particle Classifications in the PBE

- Particle classes defines how populations are represented and which physical processes must be included in the PBE model
- The framework uses three key material classes: insoluble particles, soluble particles, and dissolved species

Insoluble Particles (Noble Metals)

- Do not nucleate from solution
- Form primarily through decay process
- Do not grow or dissolve by molecular exchange
- Primarily evolve through aggregation, breakage and deposition

Soluble Particles (Corrosion Products)

- Nucleate from supersaturate solution
- Grows until saturation depletion
- Dissolves when solution is undersaturated
- **Dependence on chemical equilibrium**

Dissolved Species (Cations/Anions)

- Do not have a particle size distribution
- Transported as a dissolved concentration field
- Provide the source or sink for nucleation, growth and dissolution of soluble particles

Processes like heteroaggregation allows for class coupling

The Full Population Balance equations

Insoluble:

Soluble:

Thermochemistry and Kinetics

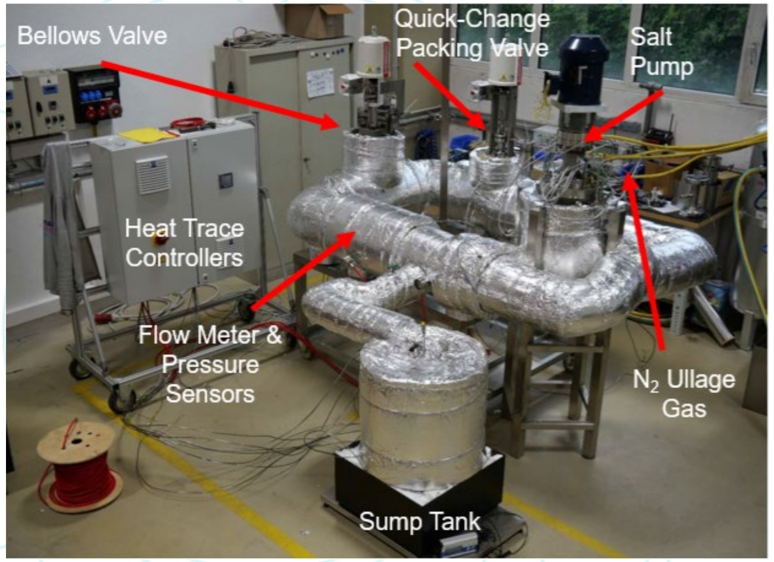
Dissolved:

Transport:

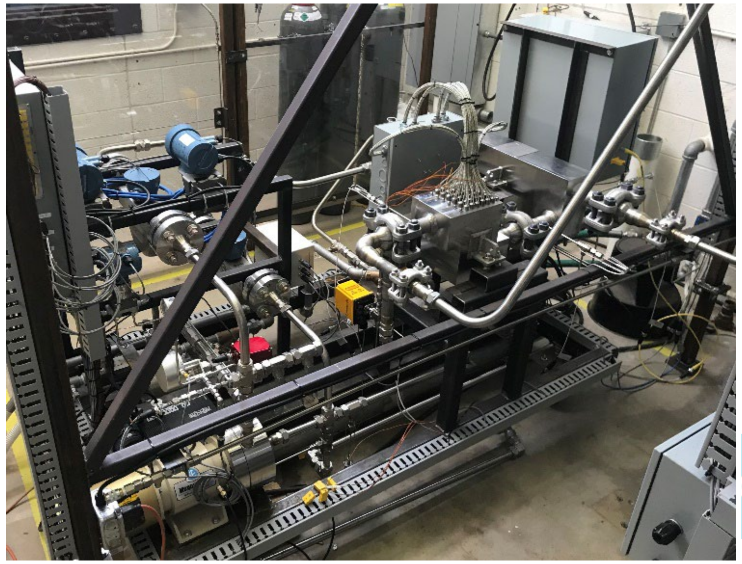
Complete multispecies transport, particle growth, deposition and decay for all present reactor species (noble metals, corrosion products, actinides)

Models Will be Tested via Super-Critical CO_2 Heat Exchanger Failure Simulation (SNL-LDRD)

- Two existing loops– a 750 °C supercritical CO_2 loop and a 750 °C salt loop- will be used
- Will use a first-of-its-kind heat exchanger designed in partnership with the University of Central Florida.
- Particulate impurities will be introduced through CO_2 ingress to create carbonates.
- Tests will be conducted at a combination of sCO_2 temperatures 300-500 °C, salt temperatures 550-750 °C, sCO2 flow rates 50-100 g/s and salt flow rates 50-100 g/s.
- Data collection will involve full system thermal-hydraulic response and monitoring of electrochemical products



Molten salt test loop



sCO_2 test loop

Parameter	Value	Unit
sCO_2 Heating Capacity	20	kW
sCO_2 Pressure	20	MPa
sCO2 Mass Flow Rate	50-250	g/s
sCO2 Op. Temp. Range	100-600	°C
Salt Heating Capacity	10	kW
Salt Pump Capacity	5-10	GPM
Salt Mass Flow Rate	50-100	g/s
Salt Op. Temp. Range	530-750	°C

Questions?

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