Molten Salt Reactor
PROGRAM

MSR Source Term Development for the MELCOR Severe Accident Code

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Annual MSR Campaign Review Meeting 22-24 April 2025

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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

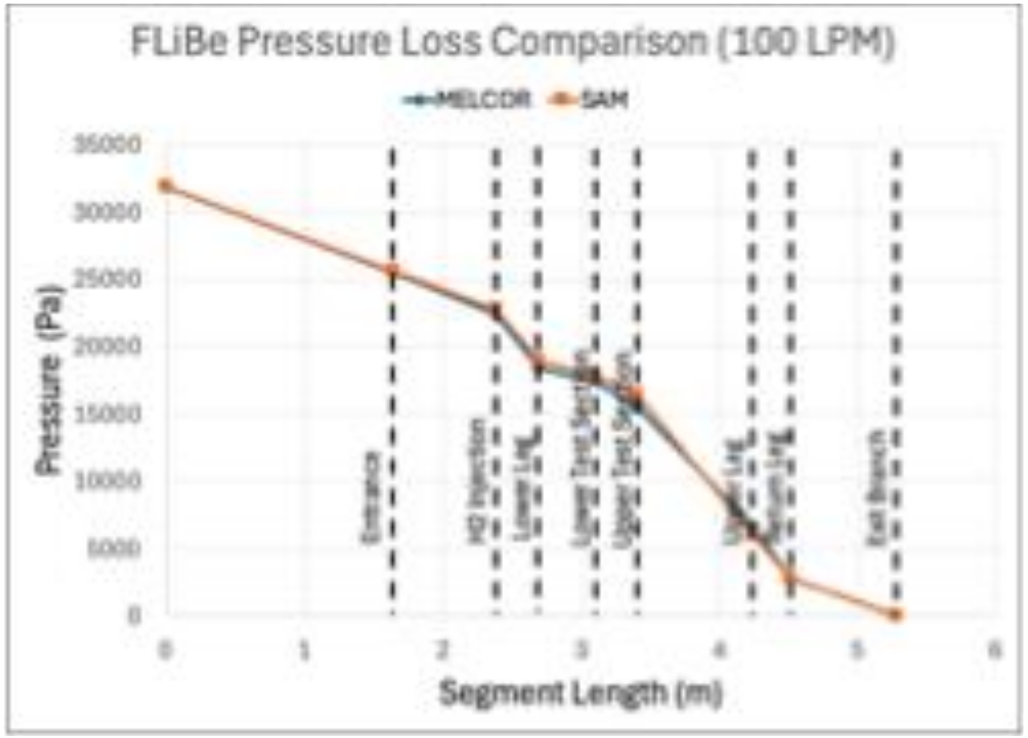
- Models constructed by user from basic components (control volumes, flow paths and heat structures)
- Demonstrated adaptability to range of reactor designs – LWR, LWR-SMR, FHR, HPR, HTGR, MSR, SFR, ATR, VVER, SFP…

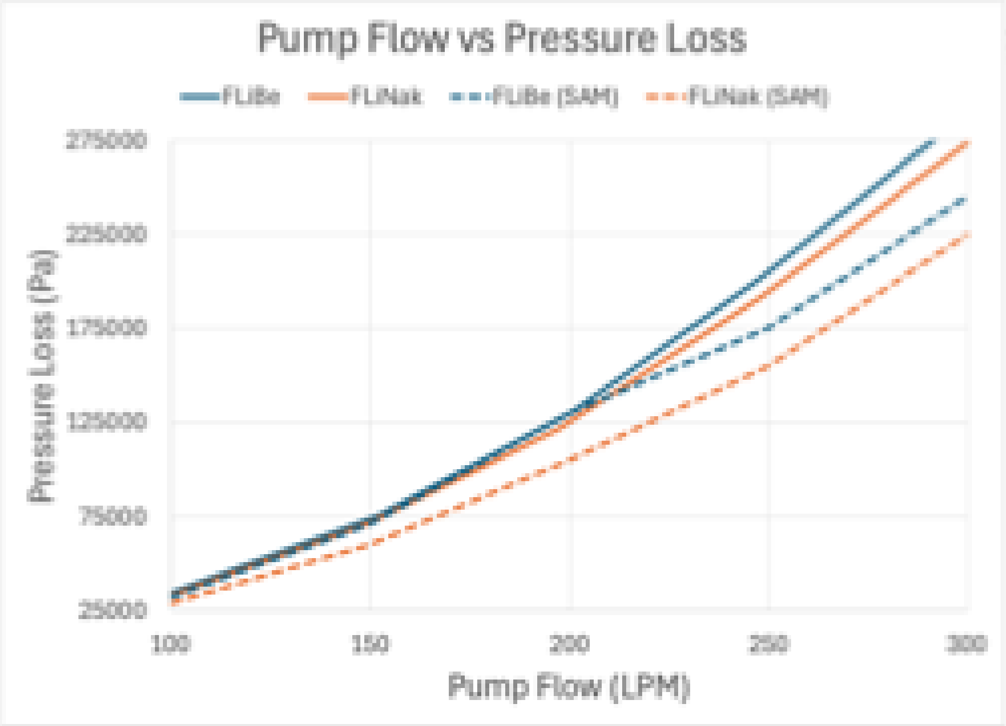
Summary of FY24 and FY25 Activities

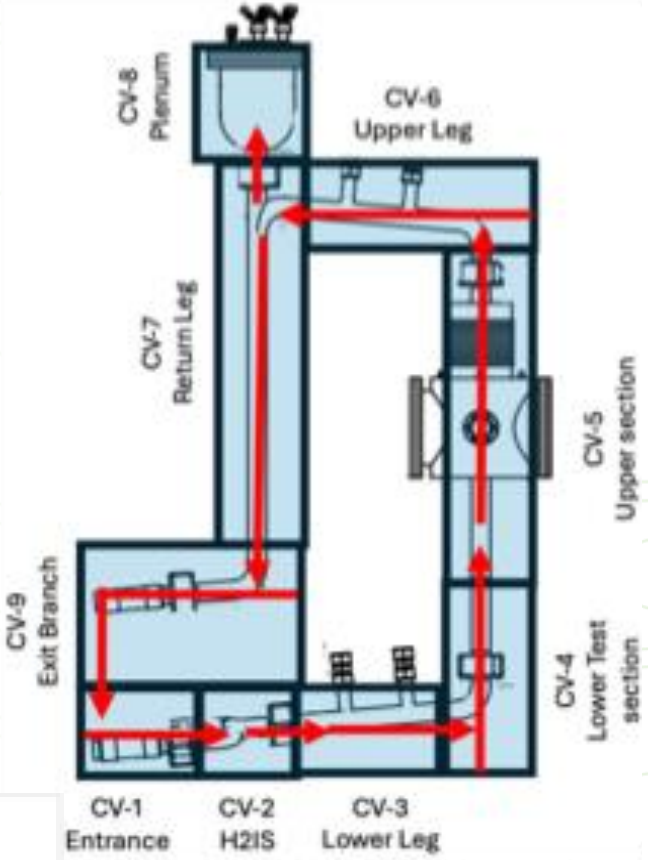
- FY2024
  - Created initial model deck for Molten Salt Tritium Transport Experiment (MSTTE)
    - Created a FLiNaK Equation-of-State (EOS) fluid model
    - Compared MELCOR results to previous SAM results
  - Updated Liquid Salt Test Loop (LSTL) model
    - Compared FLiNaK and FLiBe EOS models
    - Code-to-code comparison to SAM
  - Summary of MELCOR Chemistry Approaches
    - Discusses approach, scope and needs for modeling MSR chemistry in MELCOR
- FY2025
  - Implementing solid-deposition models into MELCOR with focus on noble metals
    - Models will include Dittus-Boelter, thermophoretic and inertial deposition modes
  - Trained a large-language model on MSRE reports with SNL ATLAS team

MSTTE Model Deck

- Created thermal hydraulic deck representation of MSTTEE using friction coefficients from previous SAM calculations[1]
- Created FLiNaK fluid file using data from U. South Carolina
- Comparison shows reproduction of SAM results for FLiBe, differs for FLiNaK
- Differences increase with higher pressures, likely due to lack of pressure response data for fluid model (compressibility, sound speed)







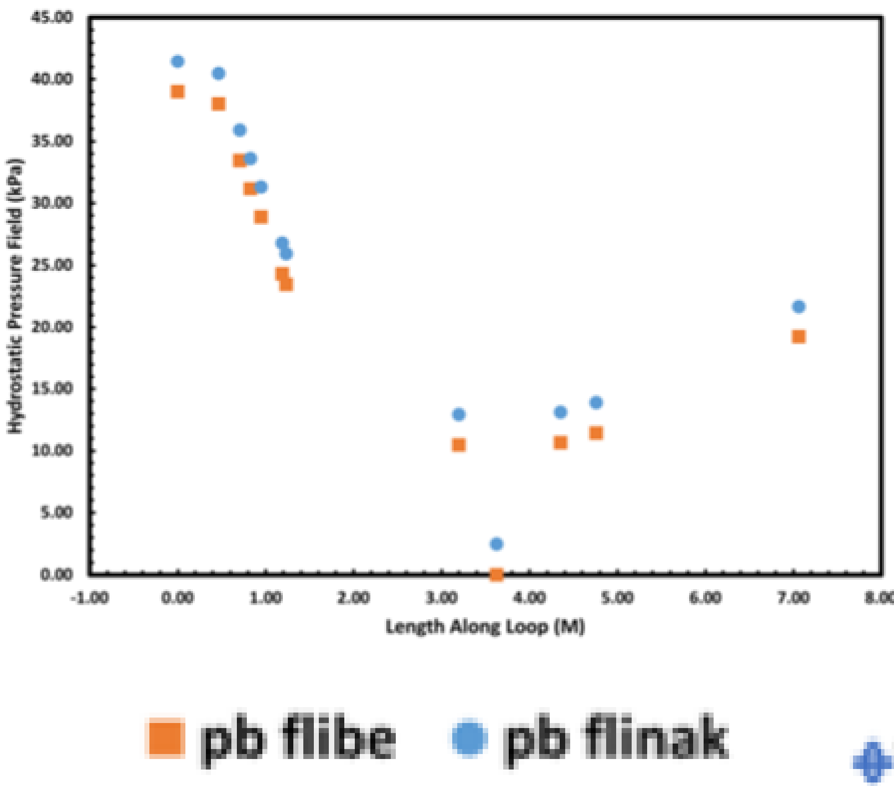
MSTTE MELCOR Model

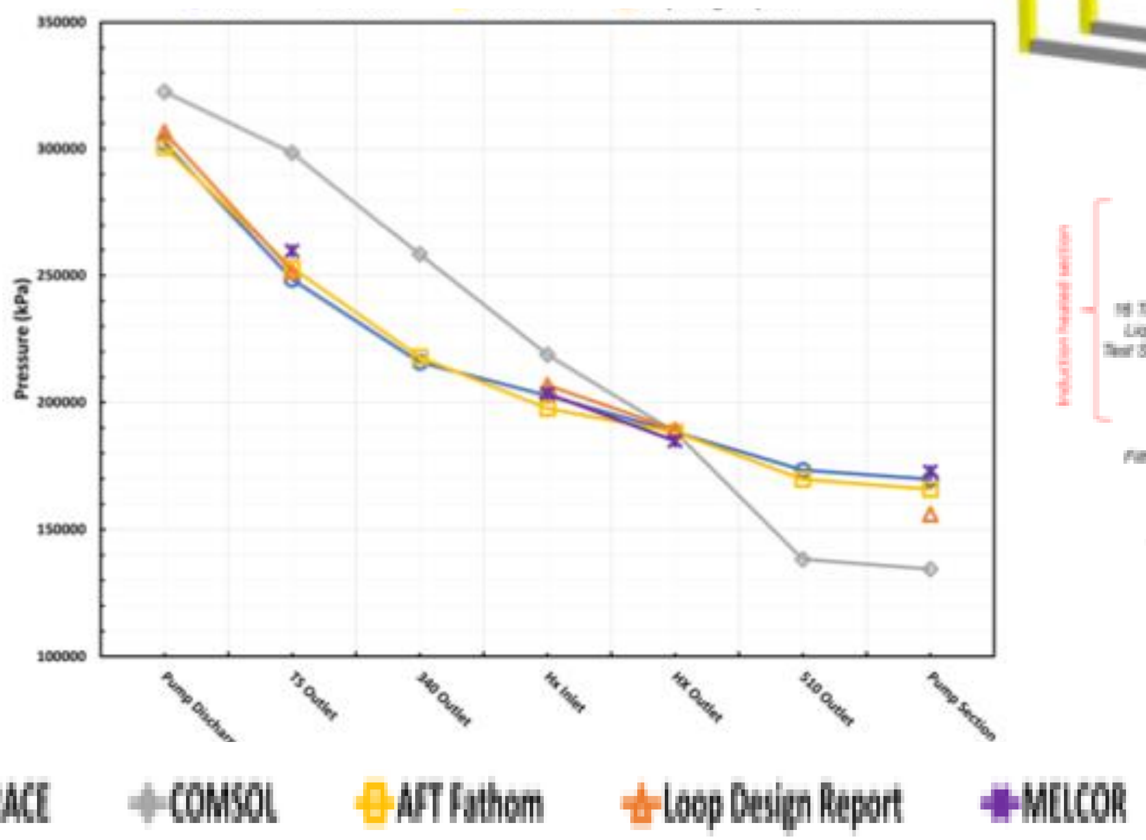
SAND-2024-12498

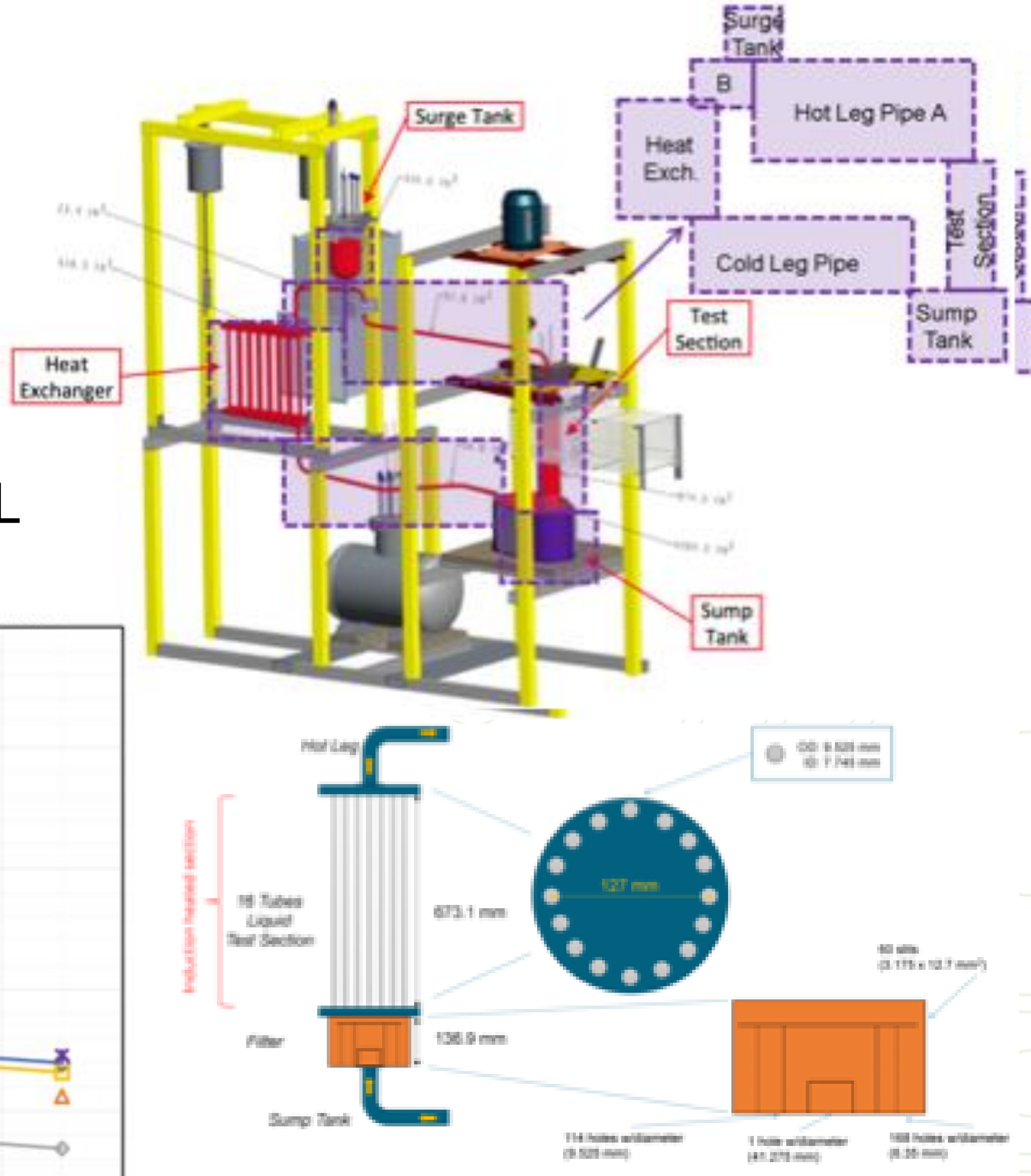
1) Fuerst, T. F. *et al.*, "Molten Salt Tritium Transport Experiment" *INL/RPT-23-74691*, 2023

LSTL Model Deck Update

- Changed test section from a pebble-bed test section to a 16-tube bundled test section
- Comparison of FLiBe and FLiNaK pressure losses are similar to MSTTE model results
- MELCOR results match well with other code simulations of LSTL







LSTL MELCOR Model
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MELCOR's MSR Chemistry Scope

- MELCOR models chemistry in COR, EOS (fluid) and in RN packages
- "Like" species are grouped to reduce computational time (e.g. Rb and Cs)
- Chemical reactions considered if equilibrium constant is $O(10^0\text{-}10^5\text{s})$
- Molten Salt Thermodynamic Database helps to model reactor's chemical speciation and create fluid files
- Can define a chemical reaction model in RN if not in MSTDB
- Models events:
  - Halogen potential control
  - Environmental contamination
  - Reactor Refueling
  - Salt Spill

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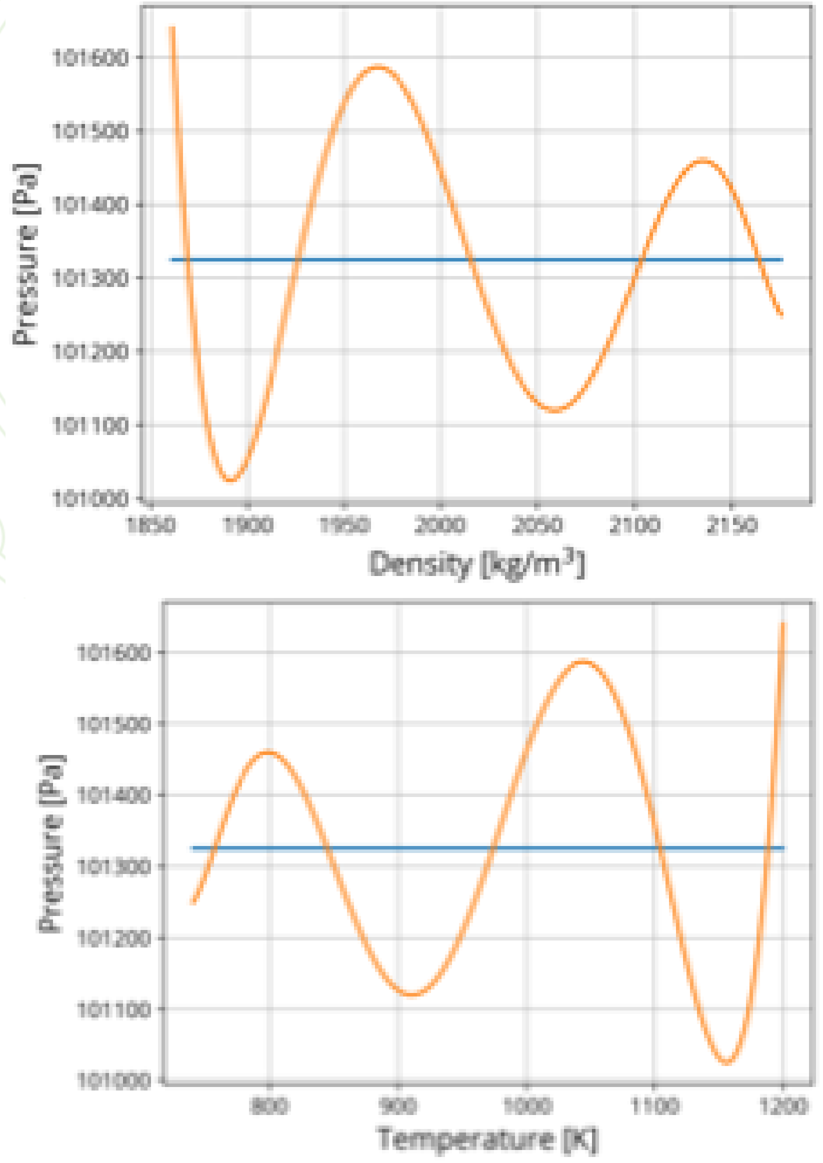
MELCOR Chemistry Road Map

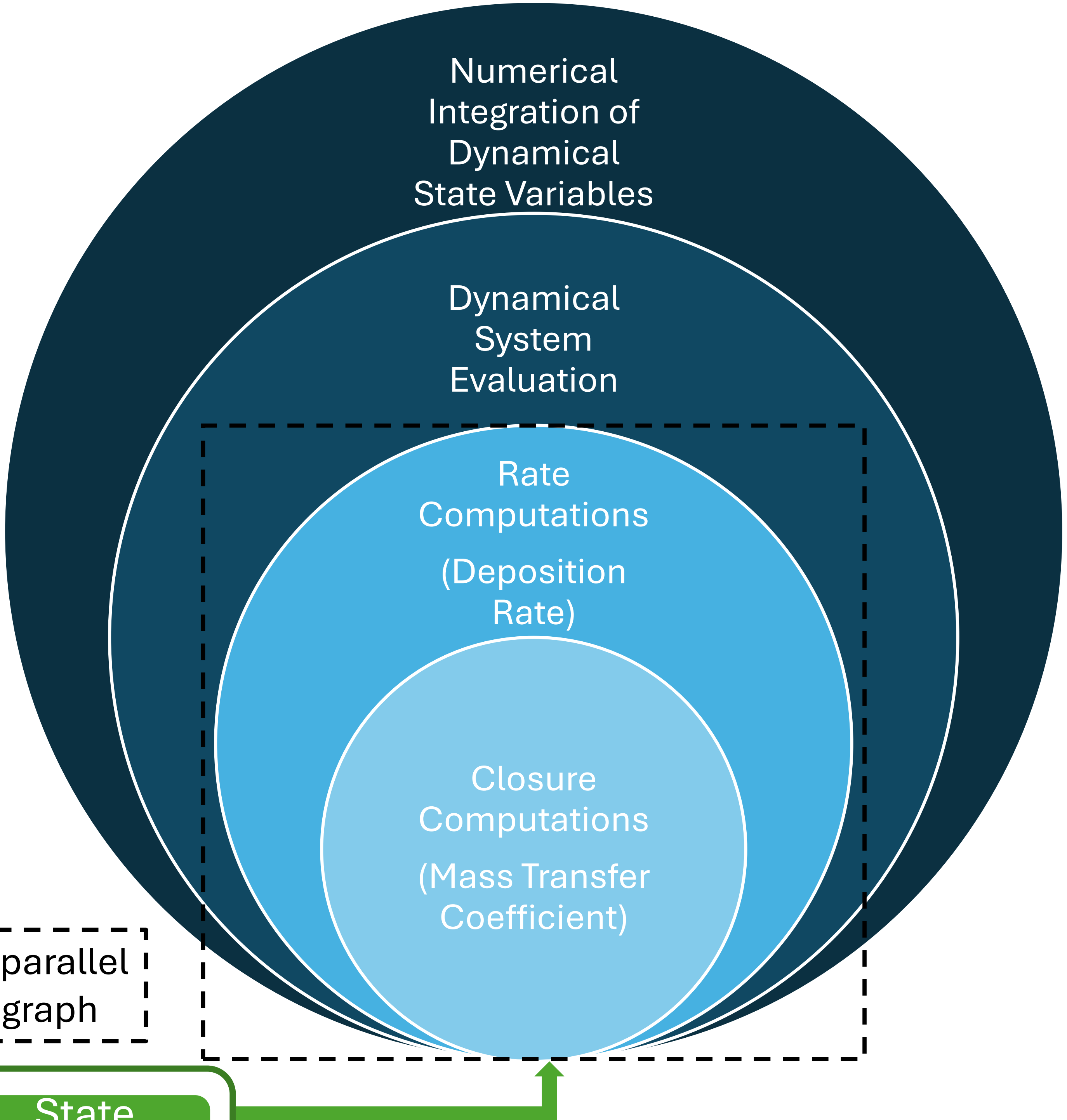
- EOS improvement requires pressure related studies
- Bubble formation and dynamics adapted from VANESA
  - Bubble size/shape
  - Diffusion through liquids and solids, such as Xe into graphite
  - Bursting transfer from liquid to vapor phases
- Adaptation of current aerosol models to MSRs
  - Salt spray/splash
- **Solid Deposition**
  - Noble metal particles
  - Corrosion products
  - Oxides from oxygen contamination

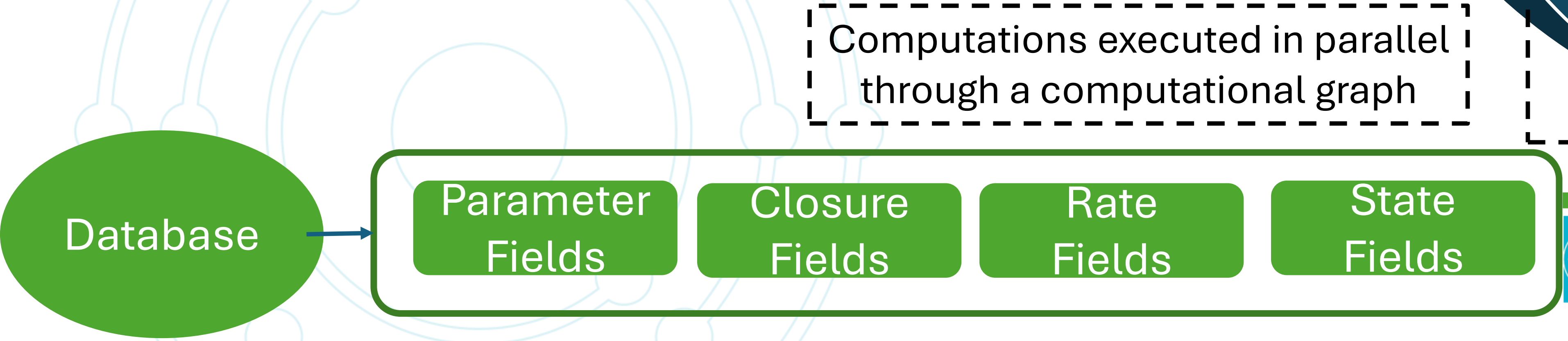


FLiNaK EOS pressure response for density and temperature

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



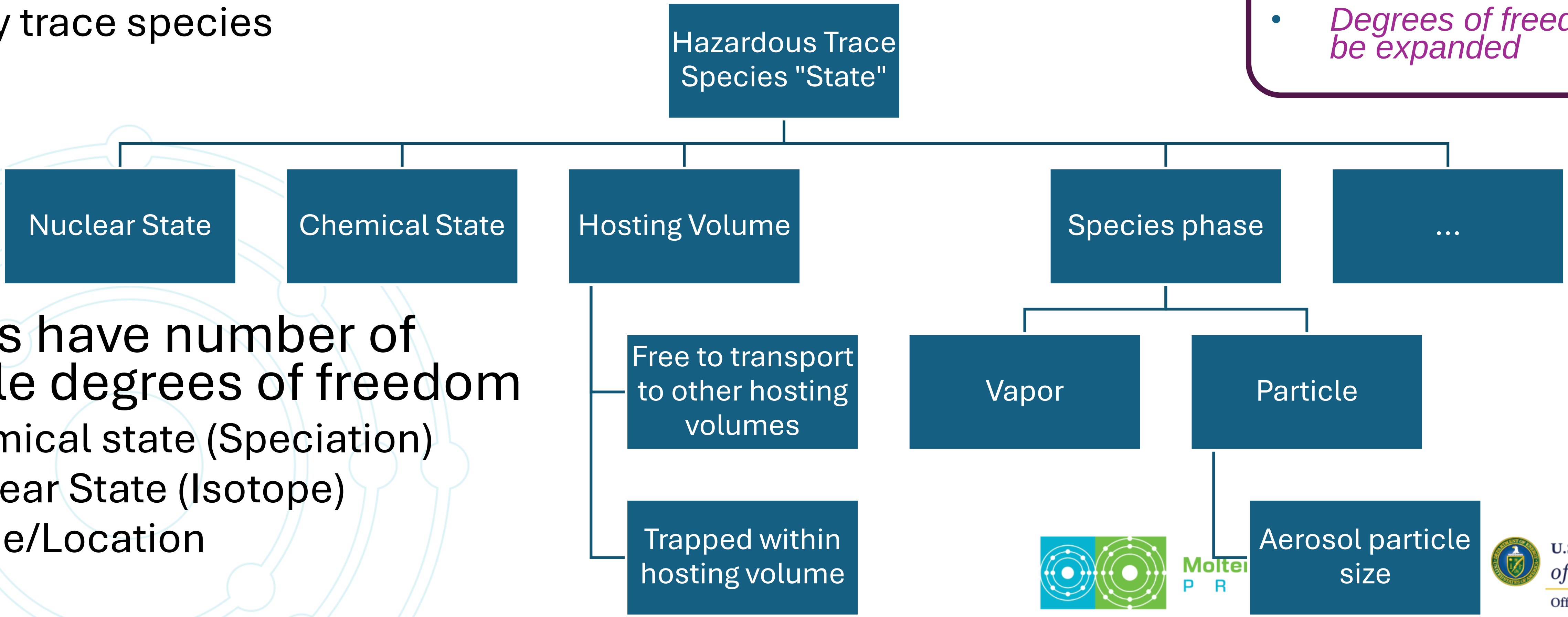


RN Package Generalized Representation of Degrees of Freedom

- 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

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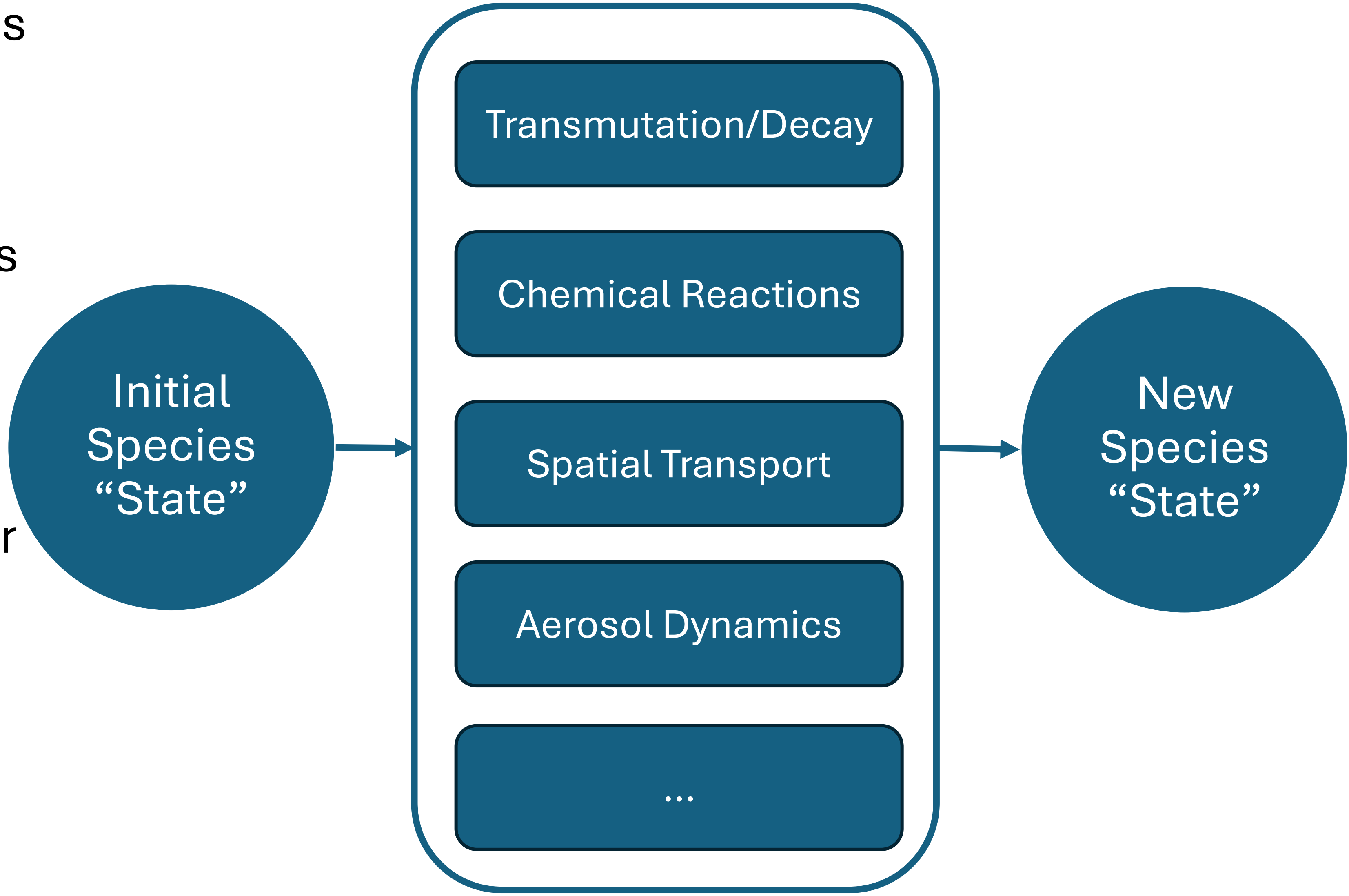
RN Package Generalized Dynamics

- 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



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

Will concentrate on initial metal deposition

Surface	Flow regime	Deposition intensity							
		^{95}Nb	^{99}Mo	^{99}Tc	^{103}Ru	^{106}Ru	^{125}Sb	^{129m}Te	^{132}Te
Surveillance specimens									
Graphite	Laminar	0.2	0.2		0.06	0.16		0.15	
	Turbulent	0.2			0.04	0.10		0.07	
Metal	Laminar	0.3	0.5		0.1	0.3			0.9
	Turbulent	0.3	1.3		0.1	0.3			2.0
Reactor components									
Graphite									
Core bar channel	Turbulent								
Bottom		0.54		0.07		0.25	0.65	0.46[a]	
Middle		1.09				1.06	1.90	0.92[a]	
Top		0.23				0.29	0.78	0.62[a]	
Metal									
Pump bowl	Turbulent	0.26		0.73	0.27	0.38	2.85	0.89[a]	
Heat exchanger shell	Turbulent	0.33		1.0	0.10	0.19	2.62	1.35[a]	
Heat exchanger tube	Turbulent	0.27		1.2	0.11	0.54	4.35	2.57[a]	
Core									
Rod thimble									
Bottom	Turbulent	1.42		1.23	1.54	0.50	3.27	1.65[a]	
Middle	Turbulent	1.00		0.73	0.58	0.42	1.35	0.54[a]	

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

Model Assumptions and Objectives*

- Assumptions
  - The system is well mixed such that the inventory of noble metals is equally distributed across the MSR
  - The reactor is not in start-up conditions
  - Metal particles transport is equal to the carrier salt flow rate during operation
  - Colloids can grow on surface, then dislodge and re-enter reactor circulation
- Objectives
  - Noble-metal fractions are "deposited" by being subtracted from the element mass in the control volume
  - A fraction of noble-metals returns to the pool after undergoing decay
  - A chemical model relating niobium solubility to redox conditions is needed for proper modeling
  - A deposited iodine fraction needs to be represented

***Generalized RN allows models to easily expand and grow in complexity to tailor to specific desired scenarios**

Dittus-Boelter Captures Diffusive and Convective Deposition

- Dittus-Boelter mass transfer depends on fluid non-dimensional numbers
- Assumes Einstein-Stokes diffusion

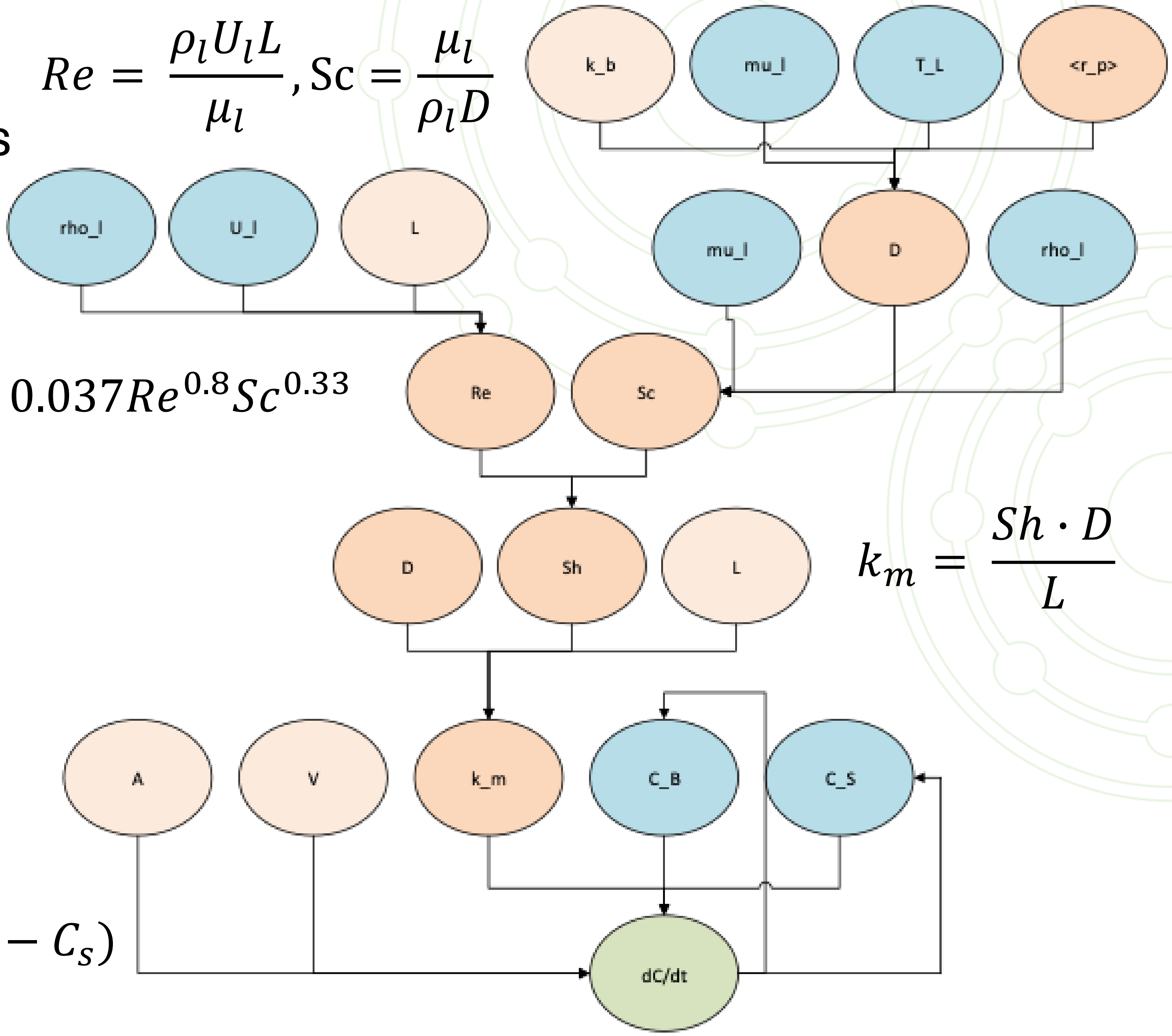
$$D = \frac{k_B T}{6\pi \mu_l r}$$

$$Re = \frac{\rho_l U_l L}{\mu_l}, Sc = \frac{\mu_l}{\rho_l D}$$

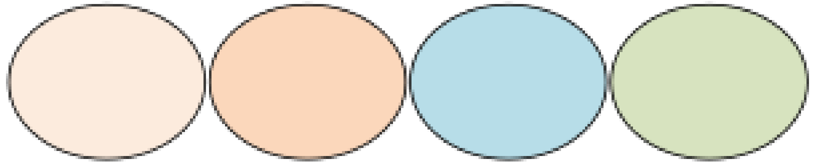
$$Sh = 0.037 Re^{0.8} Sc^{0.33}$$

$$k_m = \frac{Sh \cdot D}{L}$$

$$\frac{\partial C}{\partial t} = \frac{1}{V} k_m A (C_B - C_s)$$



parameter closure state variable rate



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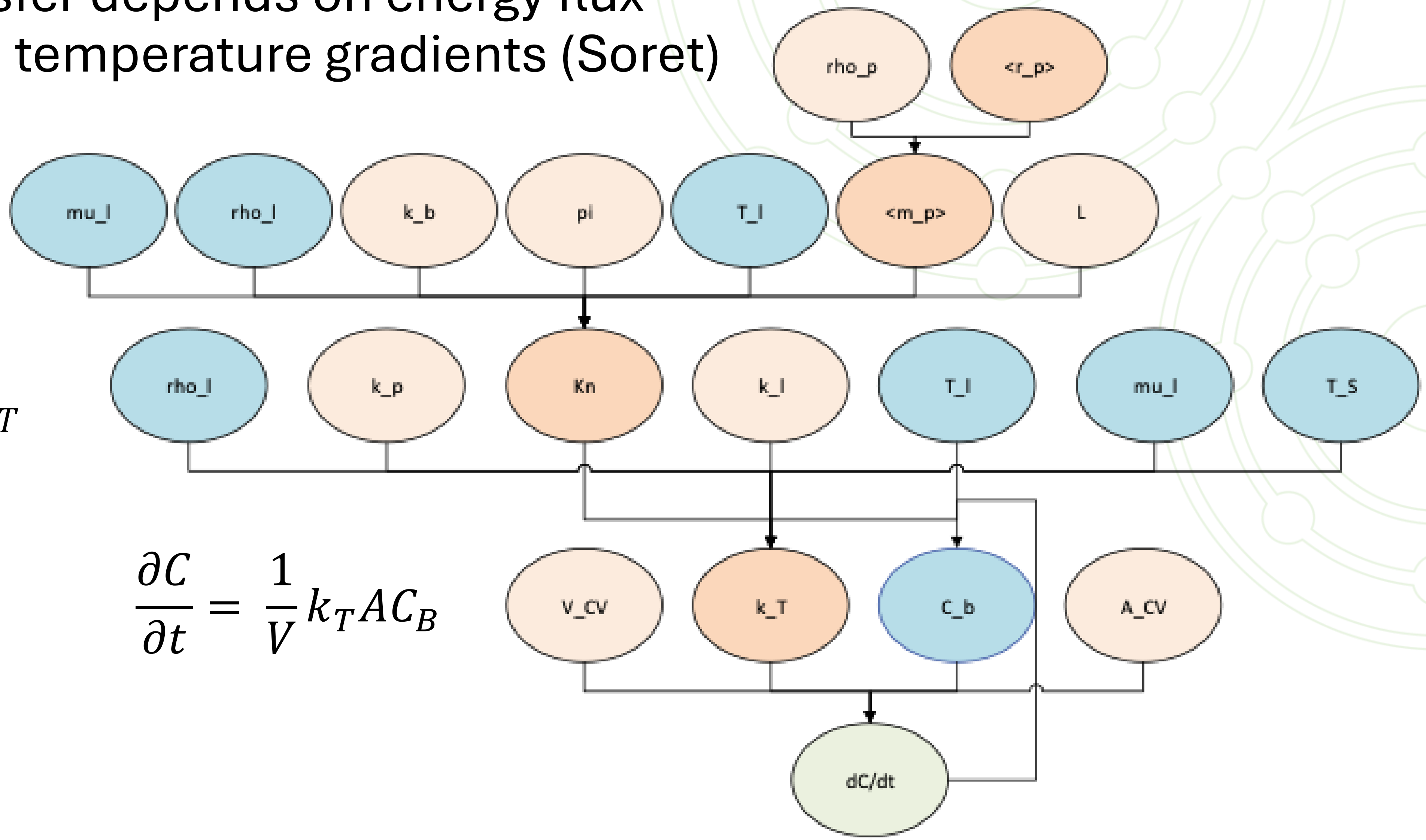
Knudsen Number Provides First-Order Approximation for Thermophoretic Deposition

- Thermophoretic mass transfer depends on energy flux (Dufour) and concentration temperature gradients (Soret)

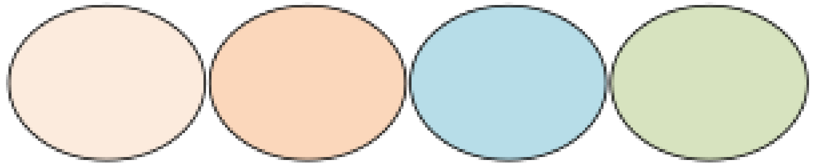
$$Kn = \frac{\mu_l}{\rho_l L}\sqrt{\frac{m_p \pi}{2 k_B T_l}}$$

$$k_T = \frac{2\mu_l(\frac{k_l}{k_p} + Kn)}{\rho_l(1 + 2Kn)(1 + 2\frac{k_l}{k_p} + 2Kn)}\nabla T$$

$$\frac{\partial C}{\partial t} = \frac{1}{V} k_T A C_B$$



parameter | closure | state variable | rate



Larger Particles have Greater Interaction with Fluid Forces

- Dittus-Boelter deposition is representative for particles smaller than 1 μm and when the particle Stoke's number, τ_p, is less than 0.2

$$\tau_p = \frac{d_p^2 \rho_p}{18 \rho_l \mu_l}$$

- The deposition velocity, V_D, in m/s for $0.2 \leq \tau_p \leq 20$

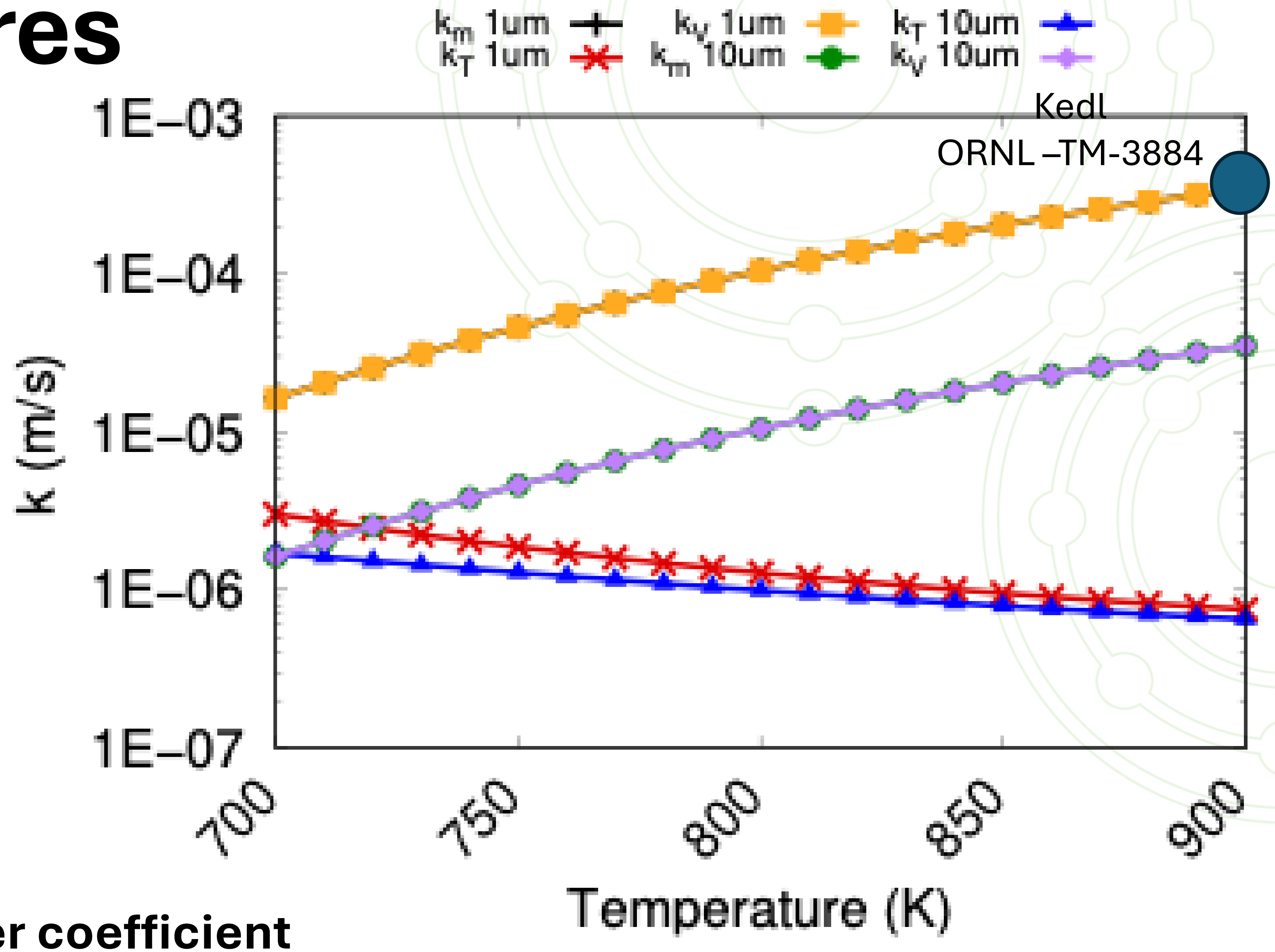
$$V_d = 4.5 \cdot 10^{-4} \tau_p^2 u^*, u^* \sqrt{\tau_0 \rho_l}$$

- For $20 \leq \tau_p, V_d = 0.13 u^*$

$$\frac{\partial C}{\partial t} = \frac{1}{V} V_d A C_B$$

Dittus-Boelter Deposition Dominates at Operating Temperatures

- Particle radius decreases mass transfer coefficient due to decreased diffusion
- Particle is in Dittus-Boelter regime because τ_p is $O10^{-4}$
- Thermophoretic deposition is inversely proportional to temperature due greater FLiNak density/viscosity



Results match Kedl's reported mass transfer coefficient

1 m pipe, 5 m/s flow in FLiNak assuming Te particle density, 300K surface temperature

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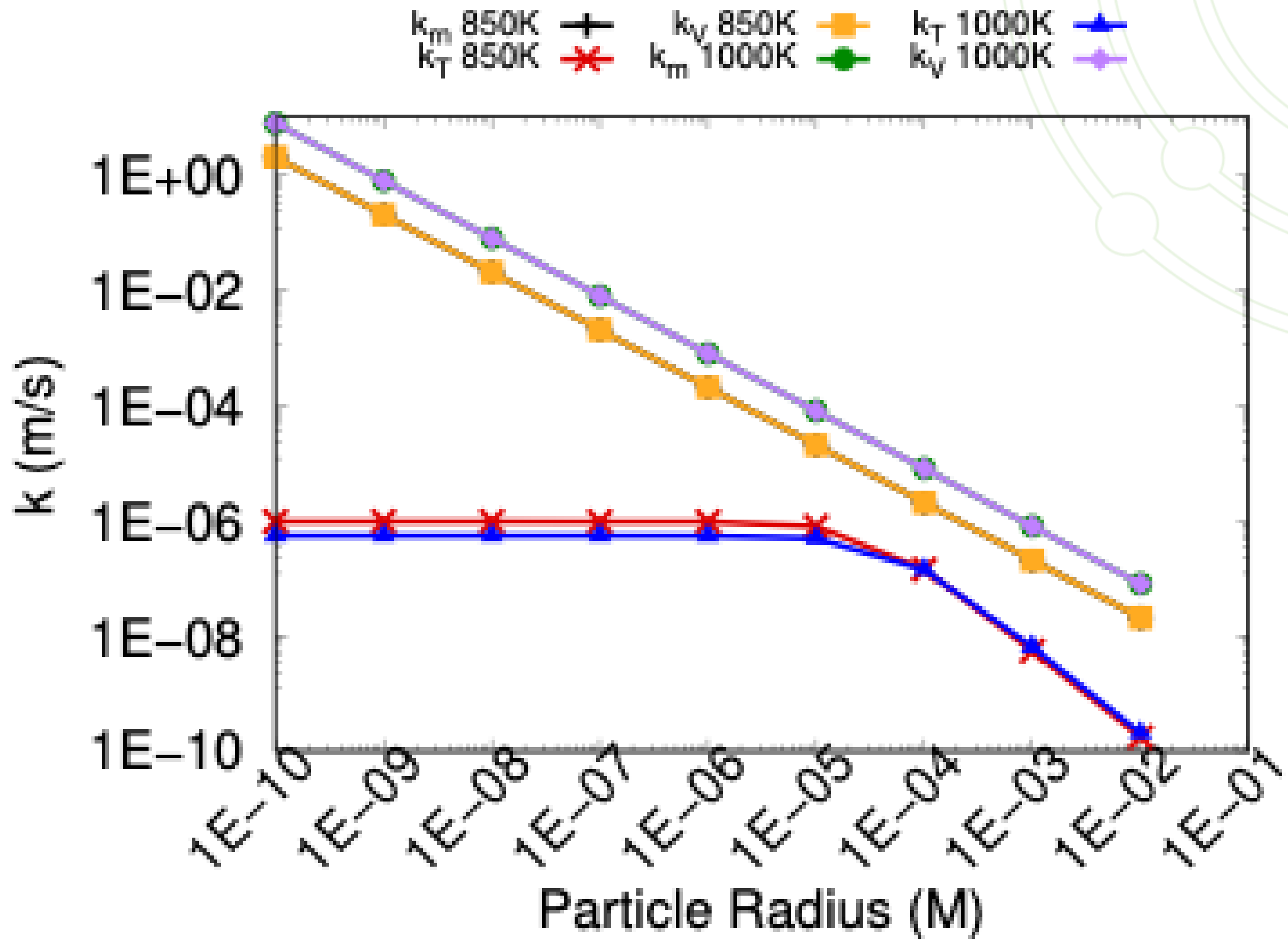
Mass Transfer Coefficients are Strongly Dependent on Particle Radius



Strong dependency on radius implies a particle growth model is needed

Implementation Status and Remaining FY25 Tasks

- Dittus-Boelter deposition is implemented along with corresponding unit tests
- Thermophoretic and velocity-based deposition will shortly be implemented
- Looking at implementing particle growth model based on models by Wilson Chiu
- Need to find a gravitational (settling) model
- Holding off on particle desorption model, but considering Arrhenius pre-factor using adsorption energies
- Will perform MSR model testing when MELCOR generalized framework becomes operational

Bonus: Worked with SNL ATLAS team to train a large-language AI model on ORNL MSR reports to create a ChatGPT like database

Abstract submission is open! www.rockymountainregion.org

BREAKING BONDS: CHEMISTRY IN THE LAND OF ENCHANTMENT

- Join members of LANL, SNL and UNM for a wide range of symposium topics
- Symposia of interest are:
  - Sensor Technologies
  - Chemical Separations
  - Nuclear Fuels and Spent Nuclear Fuel Management
  - Molten Salt Chemistry
  - Gas Capture Technologies
  - Polymers and Composites for Defense Applications
  - Cement, Clays and General Geochemistry

FY26 MSR Campaign coming to New Mexico!

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