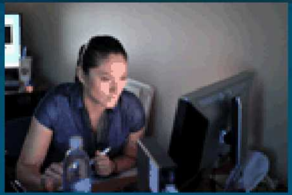
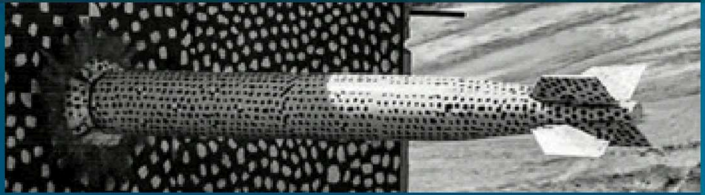
SAND2020-2736PE

MELCOR for MSRs:
Modeling, Development and Use





SNL, US NRC, CNL, CNSC, & AECL Meeting
March, 2020

PRESENTED BY

SNL Technical Staff

DEVELOPED BY

B. Beeny, L. Humphries, D. Luxat, R.Schmidt (SNL), H. Esmaili (US NRC)

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.

Overview

MELCOR molten salt reactor (MSR) and fluoride high temperature (FHR) reactor modeling

- Capabilities
- Survey of phenomena

USNRC/SNL/ORNL non-LWR evaluation model (EM) and source term demonstration calculations

Noteworthy outcomes from FY 2019 LDRD on MELCOR & MSRs

- Molten salt reactor experiment (MSRE) demonstration deck
- Conceptual circulating fuel point kinetics model (accounting for delayed neutron precursor drift)

Areas of future MELCOR development aimed at MSR/FHR

- Fission product and radionuclide transport in molten salt
- Fission product speciation and chemistry (thermochimica)

MELCOR MSR and FHR Modeling Status

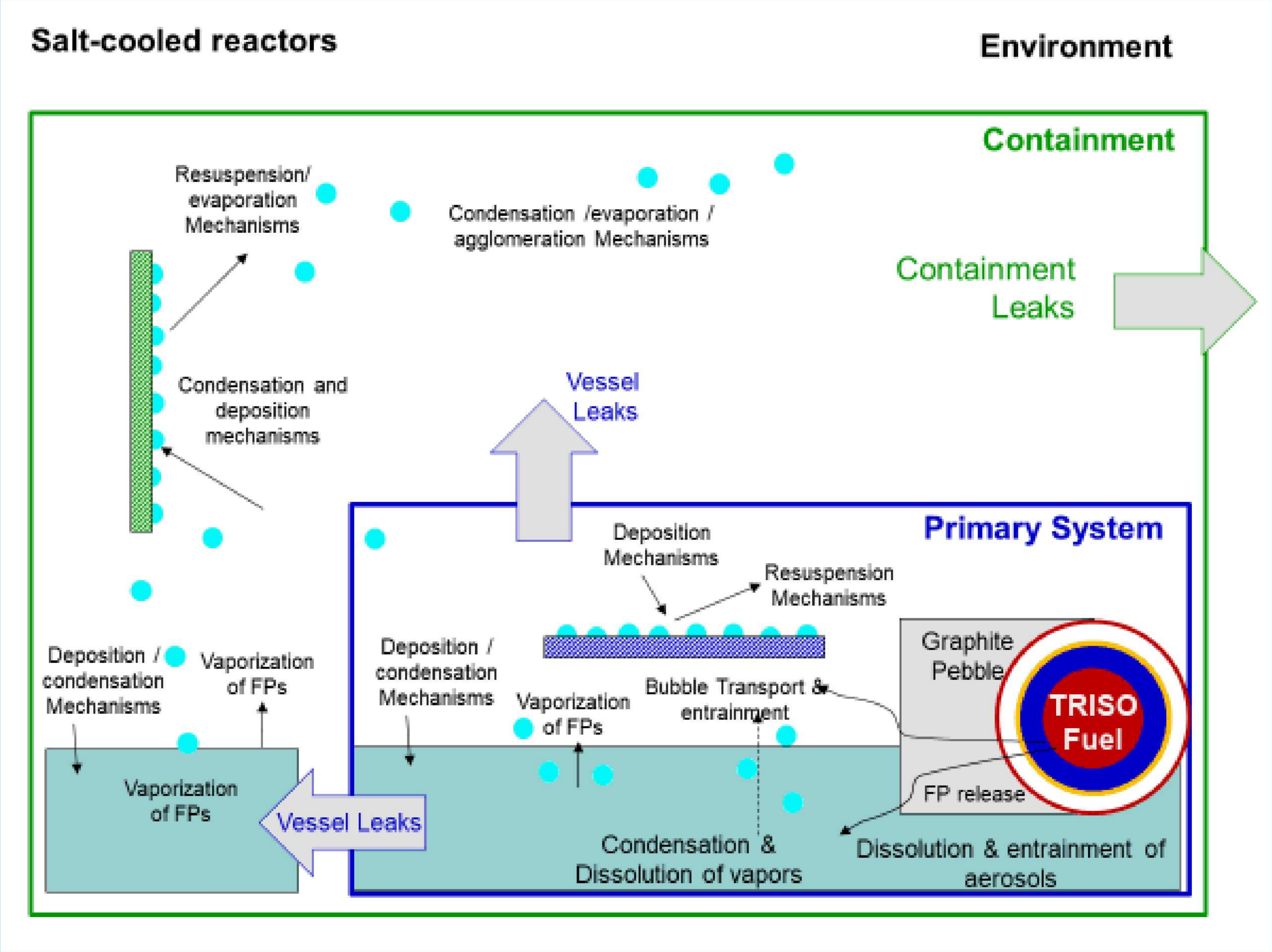
NRC and SNL actively extending MELCOR for MSR/FHR modeling
- NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy (Volume 3)
- LDRD at SNL to develop capabilities to assess safeguard/non-proliferation issues

Leverage existing capabilities
- General EOS library read-in utility (developed for sodium/SFRs) enabled FLiBe
- TRISO fuel and pebble bed models (developed for HTGRs)
- Multi-physics and flexible code architecture

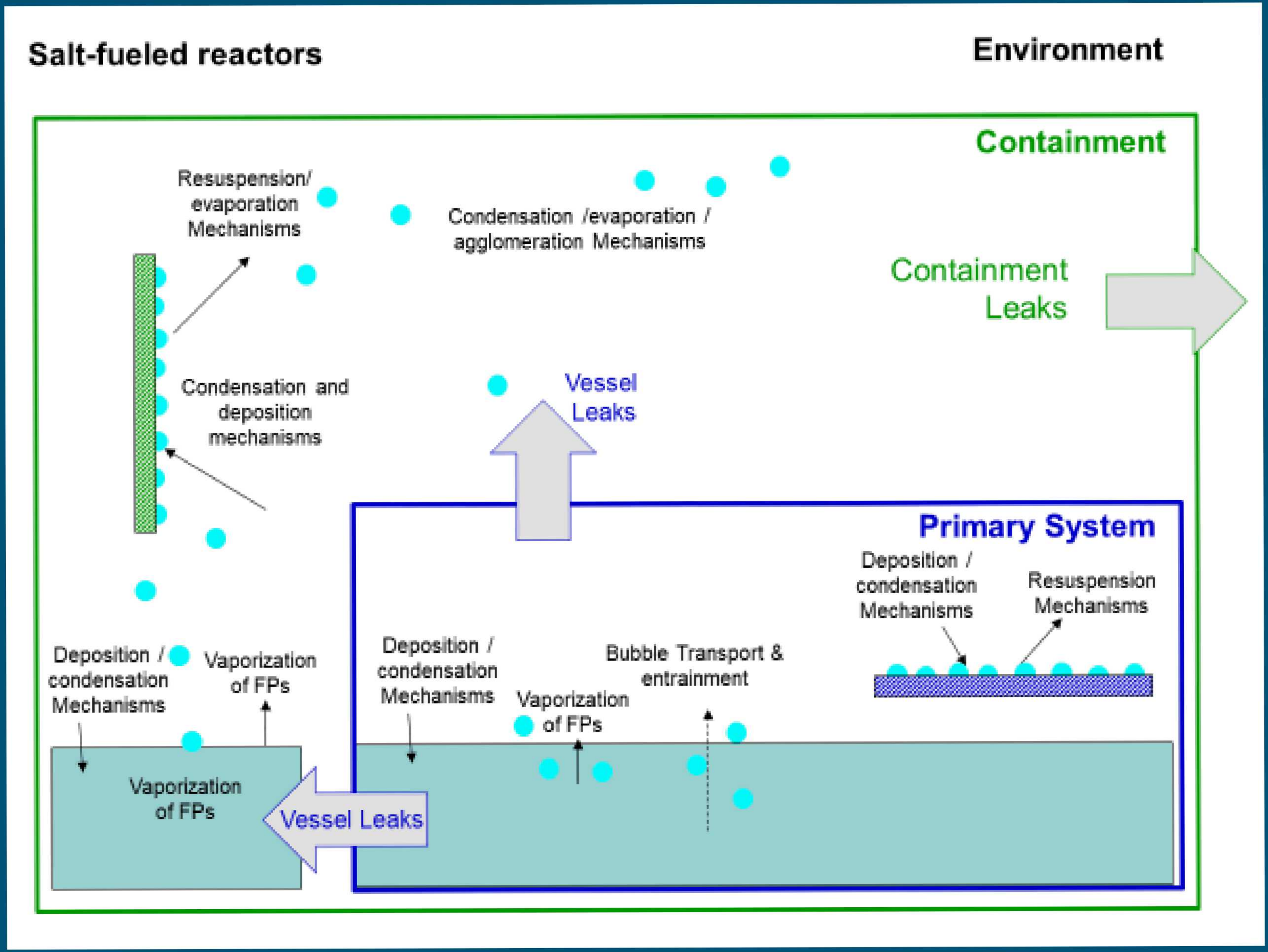
Expansion of certain capabilities (e.g. circulating fuel point kinetics)

New capabilities
- Other-than-FLiBe salts (EOS models and transport properties)
- Salt and fission product speciation/chemistry plus radionuclide transport

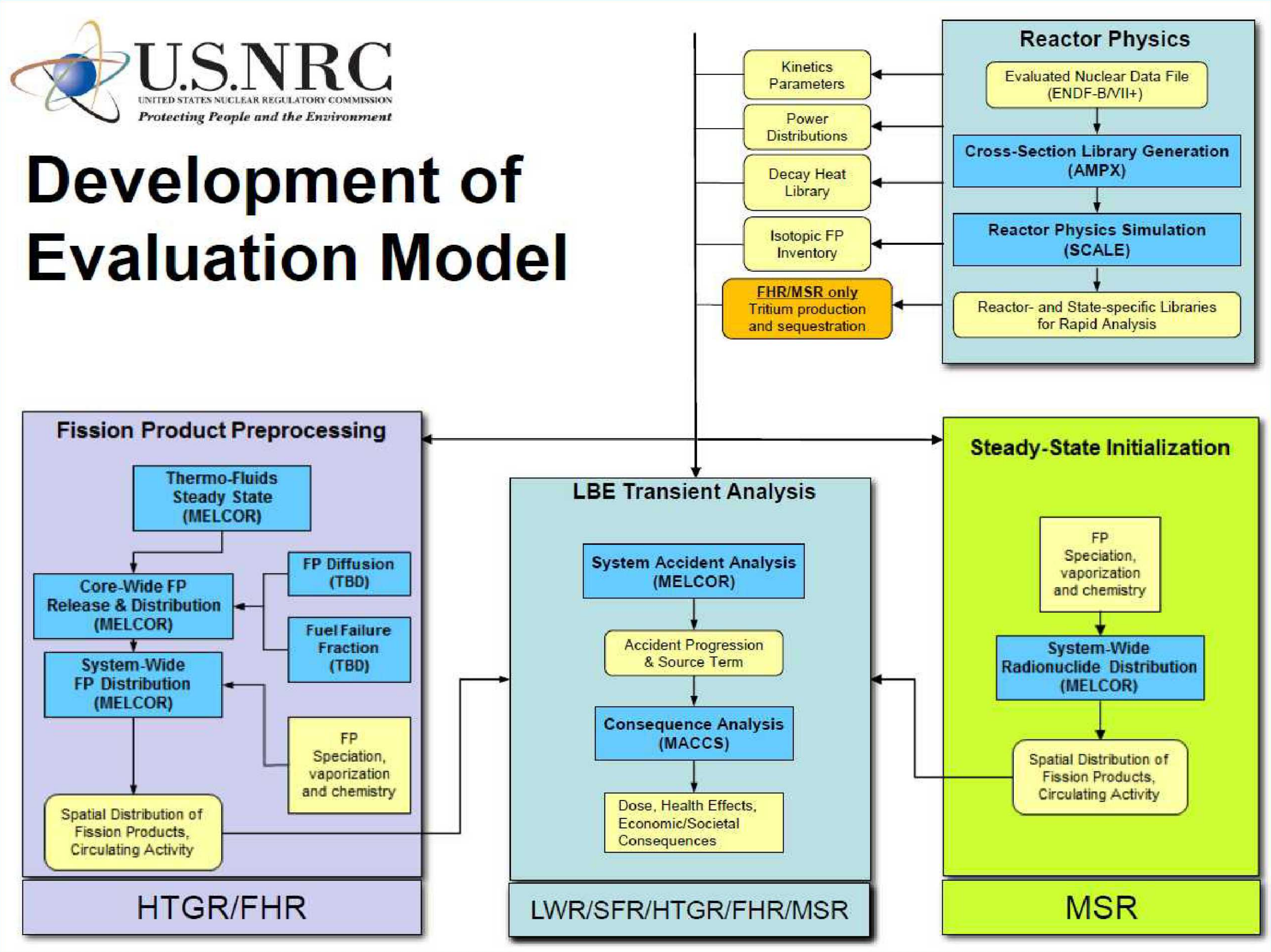
FHR Phenomena



MSR Phenomena



USNRC/SNL/ORNL Non-LWR Evaluation Model



USNRC/SNL/ORNL Source Term Demonstration Calculations

Near-term goal to complete three non-LWR source term demonstration calculations
- HTGR pebble bed using the PBR-400 reference design
- HPR using MegaPower reference design
- FHR using PB-FHR reference design

Most of the requisite capabilities are presently available in MELCOR, focus on:
- Demonstration of EM concepts (with limited MELCOR/SCALE interfacing at this stage)
- Debugging as necessary
- Generating representative, mechanistic source terms
- Outputs and results (visualization, plot file, HTML, text edits)
- Identifying potential issues with and best practices for SCALE/MELCOR interface

First-pass demonstrations will be simple in terms of input

Future iterations can build complexity and work towards fulfillment of the EMs

MSRE Model Description

MSRE model based on available information (ORNL-TM-0728)

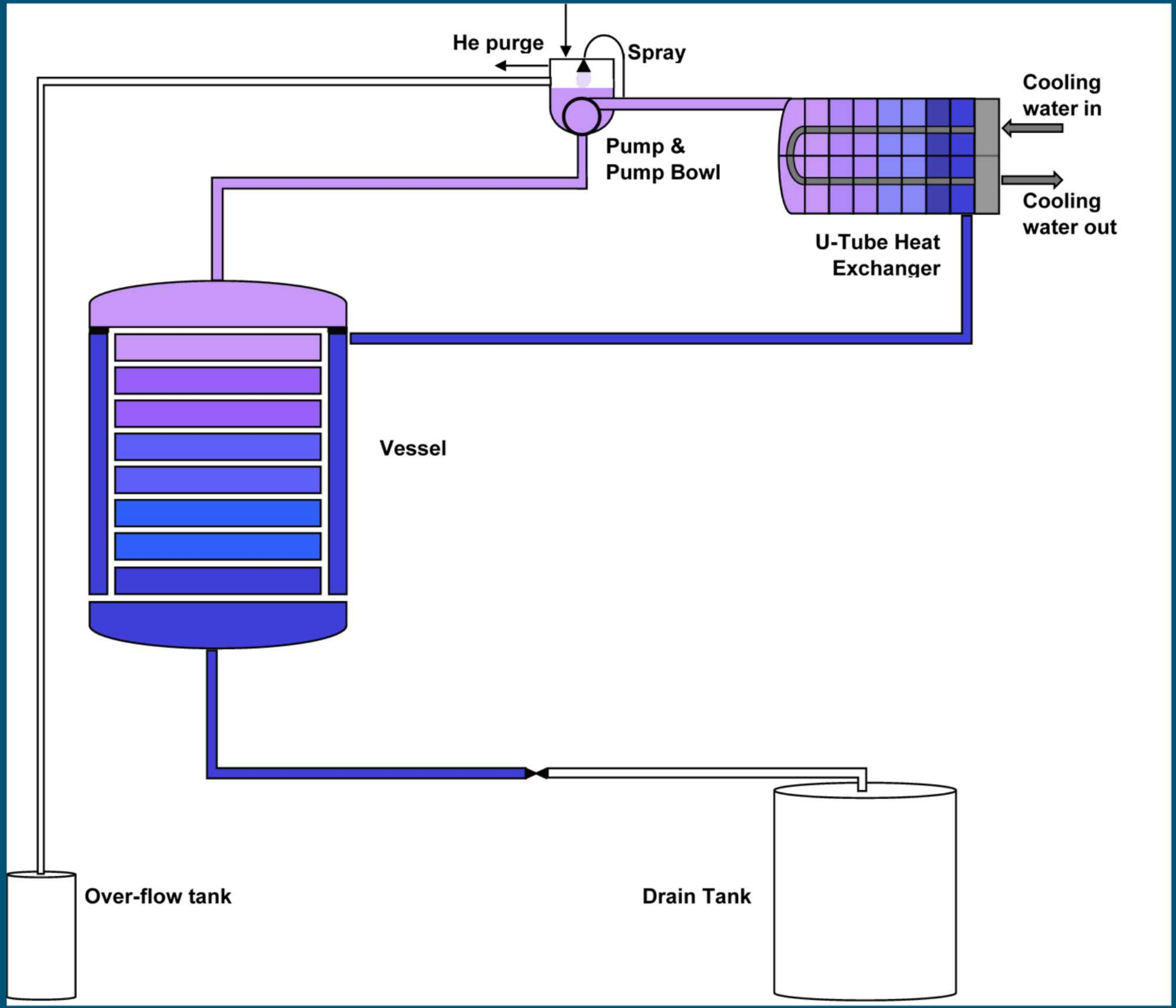
- Use currently available MELCOR models and architecture
- Could eventually demonstrate new physics models

System represented using generic MELCOR elements

- 1D core for now with 2D extension straightforward
  - 8 control volumes
  - No traditional solid core (COR)
- Graphite blocks (heat structures)
- Diversion and drain tanks in primary loop
- Core bypass (leakage flow)
- Primary loop (with heat structures for pipe walls)
- Fuel pump and pump bowl
- Horizontal u-tube heat exchanger

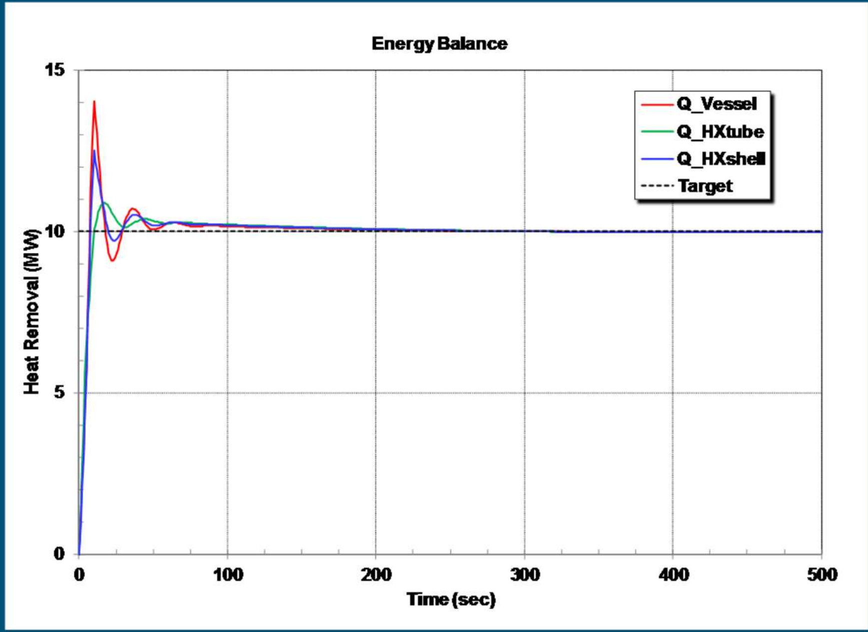
10 MWth MSRE built at ORNL in 1964 & went critical in 1965

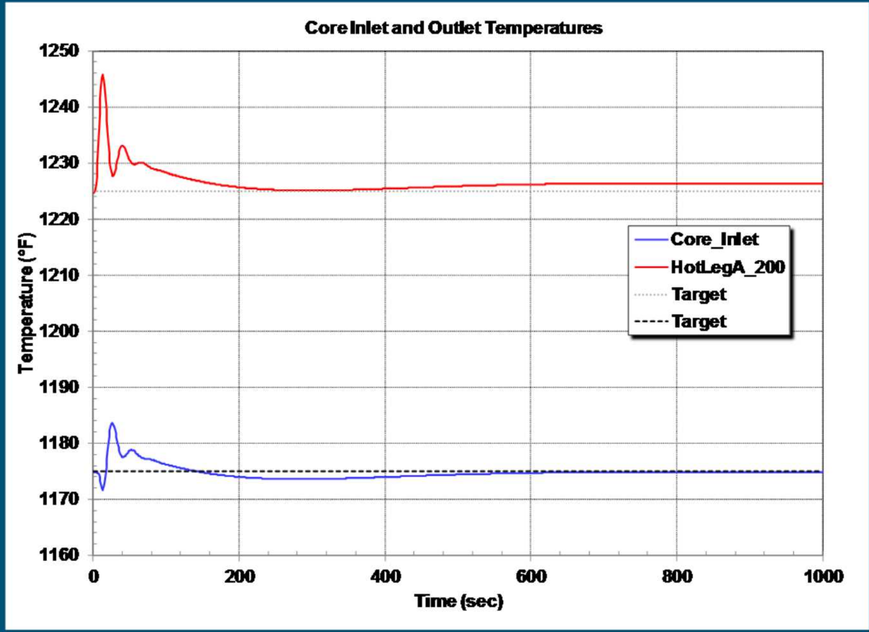
Operated until 1969 (20,000 hr)



MSRE Simulation Steady-State Results

Successful benchmarking (steady-state at nominal MSRE conditions (10 MW_{th}, T_{in}/T_{out} = 1175/1225 °F)





Initial efforts for analysis of FHR-type reactor underway

- Sample analysis based on PBR-400 (HTGR) with FLiBe as the working fluid
- Error-free execution
- Physically sensible plant response
- Will expand validation efforts

Efforts for developing source term estimates for MSR and FHR will commence in FY20

Conceptual Circulating Fuel Point Kinetics Model

Assessment

- MELCOR2 PRKE model currently applies to conventional, stationary, solid fuel
- Nuclear data for thermal, ^{235}U-fueled systems
- Certain reactivity feedback models (data from separate neutronics calculations)
- Special technique to approximate a matrix exponential and deal PRKE stiffness
- Require modifications to capture circulating fuel effects and delayed neutron precursor drift
- Require other source code "rewiring" due to when/how the solid-fuel PRKE model is implemented

Proposal(s)

- Take a lumped approach to delayed neutron precursor accounting – divide the DNP inventory "in-core" and "ex-core"
- New model with conservation equations capturing precursor "drift" (to/from) "in-core" (from/to) "ex-core"
- Apply similar numerical solution strategy to that of the solid fuel PRKEs

Mathematical formulation derived and some required code input/architecture changes already made

Conceptual Circulating Fuel Point Kinetics Model

$$\frac{dP}{dt} = \left(\frac{\rho - \beta}{\Lambda}\right) P + \sum_{i=1}^{6} \lambda_i Y_i + S_0$$

$$\frac{dY_i}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P - \lambda_i C_i, \qquad for\ i = 1 \dots 6$$

Where:

P= Thermal power due to fission

Y_i= Thermal power due to delayed neutron precursor group i

S_0= Thermal power generation rate due to neutron source

$\rho = \frac{k-1}{k}$= Reactivity for k the effective multiplication factor

β= Delayed neutron fraction

$\Lambda = {}^{1}/_{\nu V \Sigma_f}$= Neutron generation time

λ_i= Decay constant of delayed neutron precursor group i

$$\frac{dP(t)}{dt} = \left(\frac{\rho(t) - \bar{\beta}}{\Lambda}\right) P(t) + \sum_{i=1}^{6} \lambda_i C_i^C + S_0$$

$$\frac{dC_i^C(t)}{dt} = \left(\frac{\beta_i}{\Lambda}\right) P(t) - \left(\lambda_i + {}^{1}/_{\tau_C}\right) C_i^C(t) + \left(\frac{V_L}{\tau_L V_C}\right) C_i^L(t - \tau_L), \qquad for\ i = 1 \dots 6$$

$$\frac{dC_i^L(t)}{dt} = \left(\frac{V_C}{\tau_C V_L}\right) C_i^C(t) - \left(\lambda_i + {}^{1}/_{\tau_L}\right) C_i^L(t), \qquad for\ i = 1 \dots 6$$

$$\bar{\beta} = \beta - \left(\frac{\Lambda}{P(t)}\right) \sum^{6} \lambda_i C_i^L(t)$$

Where:

$P(t)$= Thermal power due to fission

C_i^C= delayed neutron precursor group i inventory/concentration in-core

C_i^L= delayed neutron precursor group i inventory/concentration ex-core (in loop)

S_0= Thermal power generation rate due to neutron source

$\rho(t) = \frac{k-1}{k}$= Reactivity for k the effective multiplication factor

$\bar{\beta}$= Effective delayed neutron fraction

β= Delayed neutron fraction (static, in absence of drift effects)

$\Lambda = {}^{1}/_{\nu V \Sigma_f}$= Neutron generation time

$\tau_{C/L} = {}^{M_{C/L}}/_{\dot{m}}$ = Residence time of precursors (core, loop, respectively)

$V_{C/L}$= Fluid volume (core, loop, respectively)

λ_i= Decay constant of delayed neutron precursor group i

Conceptual Circulating Fuel Point Kinetics Model

Revised statements of delayed neutron precursor conservation to account for drift

- In-core (core) delayed neutron precursors are:
  - Born by fission in the vessel
  - Gained by drift, i.e. transport from ex-core inventory (in-flow to core) according to loop transit time
  - Lost by decay
  - Lost by drift, i.e. transport to ex-core inventory (out-flow from core)
- Ex-core (loop) delayed neutron precursors are:
  - Gained by drift, i.e. transport from in-core inventory (in-flow to loop)
  - Lost by decay
  - Negligible gain due to delayed neutron-induced fission ex-vessel

One equation for fission thermal power magnitude, but now twelve equations for the two DNP groups

Can follow same numerical solution approach

- Cast in matricial form, but now a 13x13 coefficient matrix
- Compute/estimate a matrix exponential with the Pade(3,3) approximant
- Do same series of matrix inversions and algebraic operations

Conceptual Circulating Fuel Point Kinetics Model

A 2D spatial (r,z) distribution of DNPs at time $t + dt$ can be computed if distribution is known at time t

Within the core of a fluid-fuel reactor, delayed neutron precursor conservation may be expressed:

$$\frac{\partial C_i^C(r,z,t)}{\partial t} + v_z \frac{\partial C_i^C(r,z,t)}{\partial z} + v_r \frac{\partial C_i^C(r,z,t)}{\partial r} = \left(\frac{\beta_i}{\Lambda}\right) n(r,z,t) - \lambda_i C_i^C(r,z,t)$$

A general solution can be pursued with the method of characteristics. Treating t as a parameter, one obtains two characteristic equations:

$$\frac{dz}{dt} = v_z \,;\, \frac{dr}{dt} = v_r$$

Integrating both and allowing the constants of integration to be α and β and letting functions $A(z,t)$ and $B(r,t)$ equal those constants:

$$z(t\,;\,\alpha,\beta) = v_z t + \alpha \quad \rightarrow \quad A(z,t) = \alpha = z - v_z t$$

$$r(t\,;\,\alpha,\beta) = v_r t + \beta \quad \rightarrow \quad B(r,t) = \beta = r - v_r t$$

The PDE can be reduced to an ODE by changing coordinates to $\bar{R} = B(r,t), \bar{Z} = A(z,t), \bar{T} = t$. The resulting ODE can be integrated (integrating factor method) to yield a general solution - up to a function $F(\bar{R} = r - v_r t, \bar{Z} = z - v_z t)$ - after transforming variables back to (r,z,t) :

$$C_i^C(r,z,t) = \left({\beta_i}/{\Lambda\lambda_i}\right) n(r,z,t) + F(r - v_r t, z - v_z t) e^{-\lambda_i t}$$

In the context of this delayed neutron precursor solve, the function $n(r,z,t)$ is known. To resolve the function $F(r - v_r t, z - v_z t)$, a side condition is required. Assuming the condition:

$$C_i^C(r,z,t=0) = C_{0,i}^C(r,z)$$

Results in a solution:

$$C_i^C(r,z,t) = \left(\frac{\beta_i n(r,z,t)}{\lambda_i \Lambda}\right)\left(1 - e^{-\lambda_i t}\right) + C_{0,i}^C(r - v_r t, z - v_z t) e^{-\lambda_i t}$$

Practically, this could be used in tandem with the lumped-parameter circulating fuel PRKE solution to discern the delayed neutron precursor distribution in-core. Note that $C_i^C(r,z,t)$ and $C_i^C(t)$ from the PRKE solution are related as:

$$C_i^C(t) = \iiint_{V_{core}} C_i^C(r,z,t)\,dV = 2\pi \int_0^H \int_0^R C_i^C(r,z,t)\, r\,dr\,dz$$

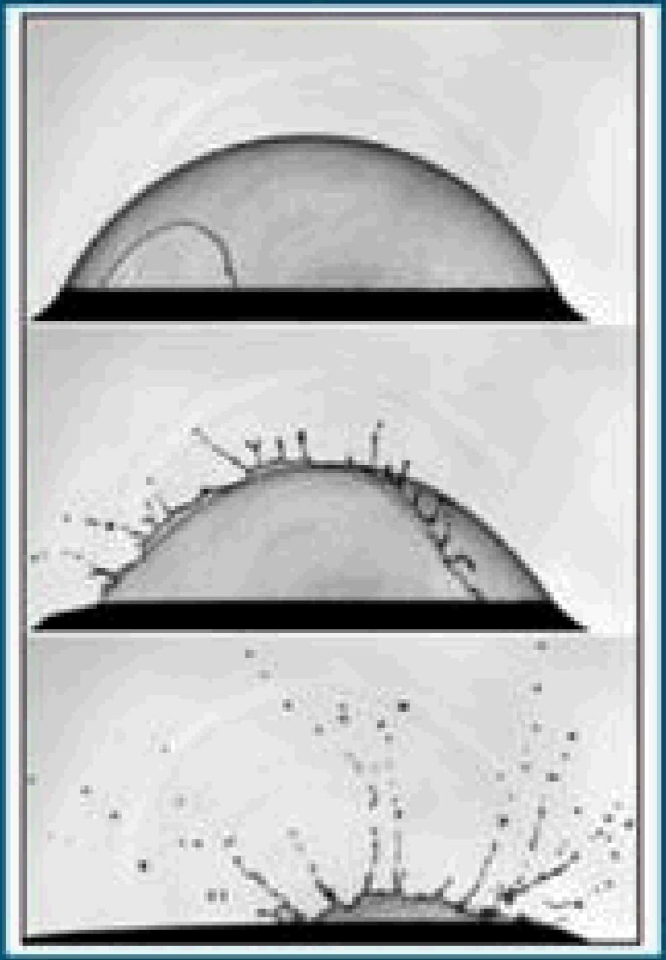
Future Code Development Areas

Fission product (radionuclide) transport in molten salt

- On-going development of fission product transport modeling (Fred Gelbard)
- Several outstanding questions
  - Appropriateness of equilibrium assumptions
  - Fission product vapor/aerosol bubble transport in molten salt pool, migration to and vaporization at a free interface
  - Aerosol (micron-sized) formation from bubble burst at free surface

Fission product (radionuclide) speciation/chemistry in/with molten salt

- Thermochimica (thermochemical equilibrium solver) a useful tool in this respect?
- New/revised capabilities for RN class transitions according to chemical transformation



Lhuissier, H and Vilermau, E. "Bursting bubble aerosols," J Fluid Mech (2012), vol 696, pp 5-44