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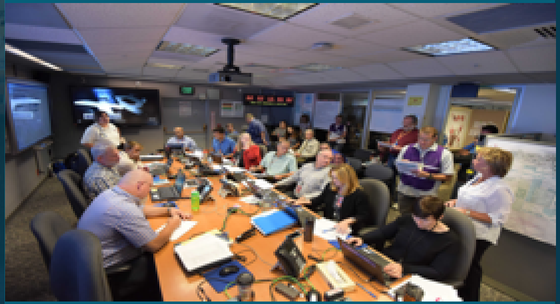
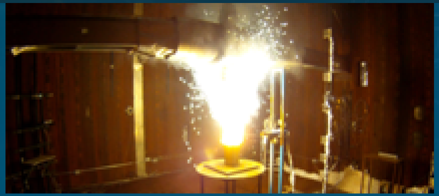
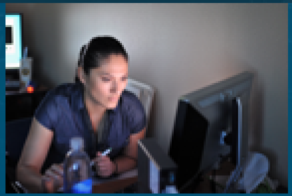
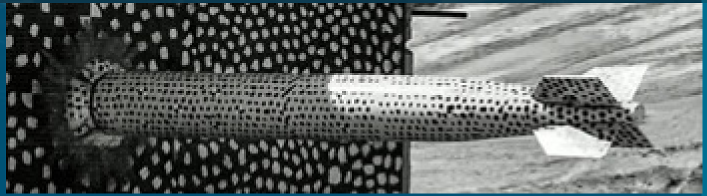


MELCOR for Molten Salt Reactor Modeling

MELCOR Workshop June 13-17, 2022

PRESENTED BY

Brad Beeny

U.S. DEPARTMENT OF ENERGY NNSA

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Overview

MSR thermal hydraulics theory

- No COR package activity
- CVH, FL, HS, and DCH/RN1
- CVH/EOS for FLiBe as a working fluid
- Fluid core in CVH
- Fluid fuel point reactor kinetics equations (FFPRKEs)

MSR thermal hydraulics practice

- Input structures
  - FLiBe EOS
  - CVH fluid core
  - CVH fluid fuel point reactor kinetics equations
- Example : Zero-power MSRE flow coast-down experimental benchmark

Conclusions

MELCOR MSR
Modeling and Development
Thermal Hydraulics – Theory

Physics Package Roles

COR package has no role

- No solid fuel structure to retain and/or release class mass to CVH/RN1
- Functions traditionally performed by COR are instead handled by CVH

CVH/FL does fluid core thermal hydraulics modeling

- FLiBe equation-of-state,
- Fission power generation,
- Hydraulic solution,
- Fluid fuel point kinetics for power/flow dynamics

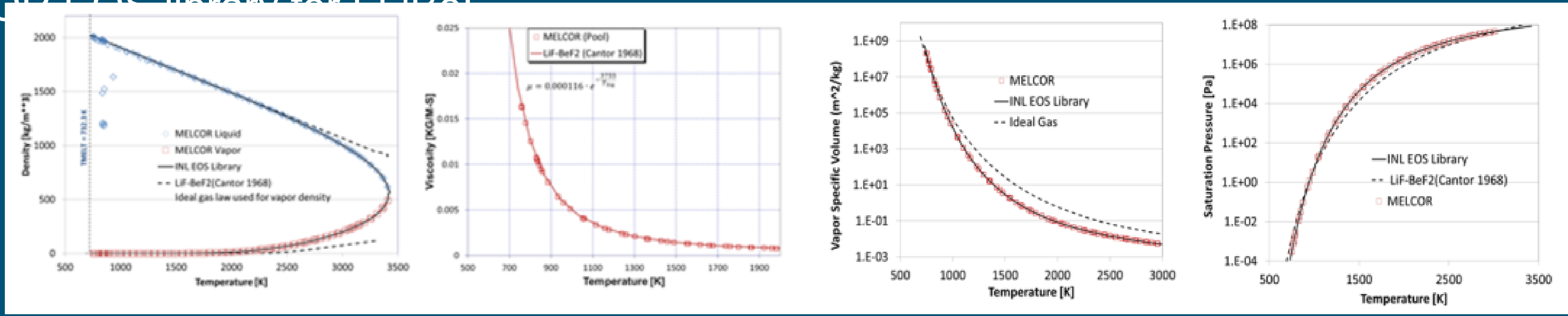
HS represents any solid structures in/around/about the fluid core region

DCH for class specific decay power and CVH/RN1 (GRTR) for form-wise class mass tracking

CVH and FLiBe EOS

Generic working fluid EOS libraries – originally added for sodium - expanded for molten salts (FLiBe)

- INL fusion safety program developed alternate fluid property data files for a multi-fluid EOS approach, used in MELCOR
- Chen’s soft sphere model (sodium) modified for FLiBe (Humrickhouse & Merrill - INL/EXT-17-44148 – 2017)
- Property database from ORNL data (Cantor – ORNL-TM-2316 – 1968)
- Verification of MELCOR EOS library for FLiBe:
  - Single CV tests case
  - Internal energy source
  - At saturation
  - Verified properties too



Limited validation activity against ORNL MSRE

Recent EOS model developments focus on special cases (e.g. approach to freezing, FLiBe vapor formation)

CVH Fluid Core

Define a fluid core from CVs including:

- A type associate denoting “core” CVs and “loop” CVs
  - “Core” CVs comprise a portion of the active core
  - “Loop” CVs comprise a portion of the primary fuel flow loop OUTSIDE the active core
- An axial and radial power distribution and power level P_0
  - Similar in concept to COR_ZP and COR_RP
  - Fixed active core power profile shape despite flowing fuel
  - Magnitude of power level from CF and/or FFPRKE predictions
- DCH and RN1 (GRTR) inputs for either or both of:
  - Initial class mass by form
  - Class mass source by form

Energy generation in “core” and “loop” CVs:

- External pool energy sources (configured internally) facilitate fission power deposition into pool phase of “core” CVs
- Typical DCH/CVH/RN1 activity facilitates decay heat deposition into pool phase of “loop” CVs

FFPRKEs - Delayed Neutrons and Reactor Kinetics

Time-dependent neutron population (kinetics) plus system feedback mechanisms (dynamics)

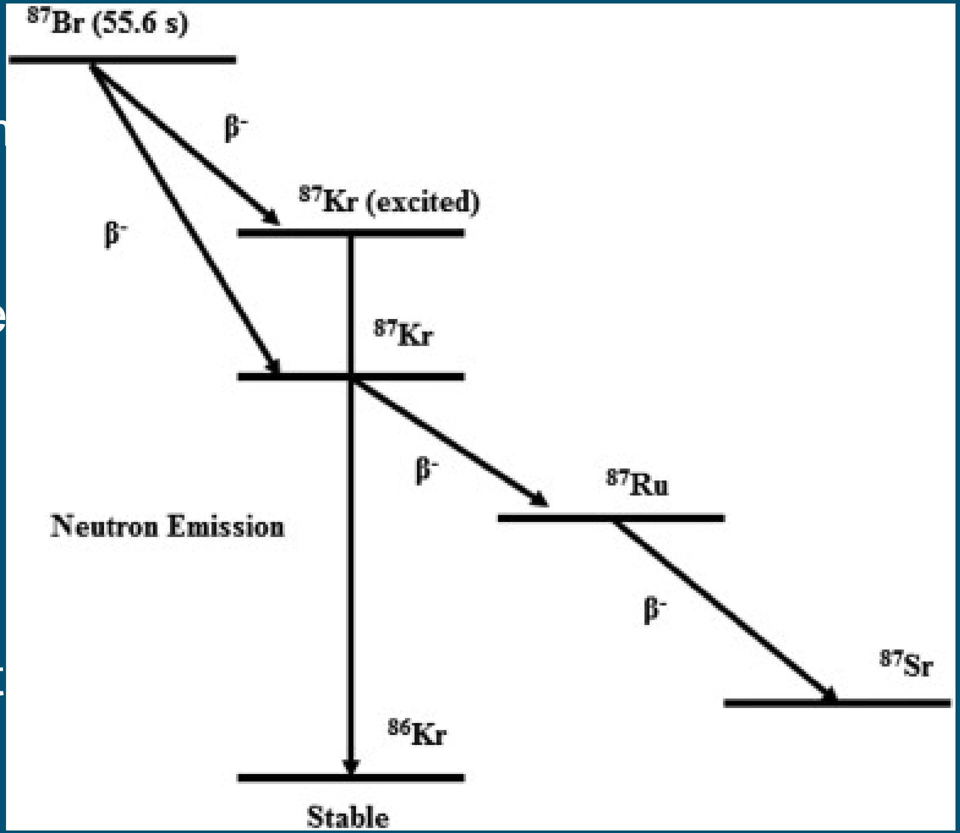
Delayed neutron (DN) emission from DN precursor (DNP) decay is a primary governor of dynamic response

- Solid fuel –DNP's stay and hence DN's contribute to economy
- Fluid fuel – DNP's move (ex-core) and lost DN's impact econon

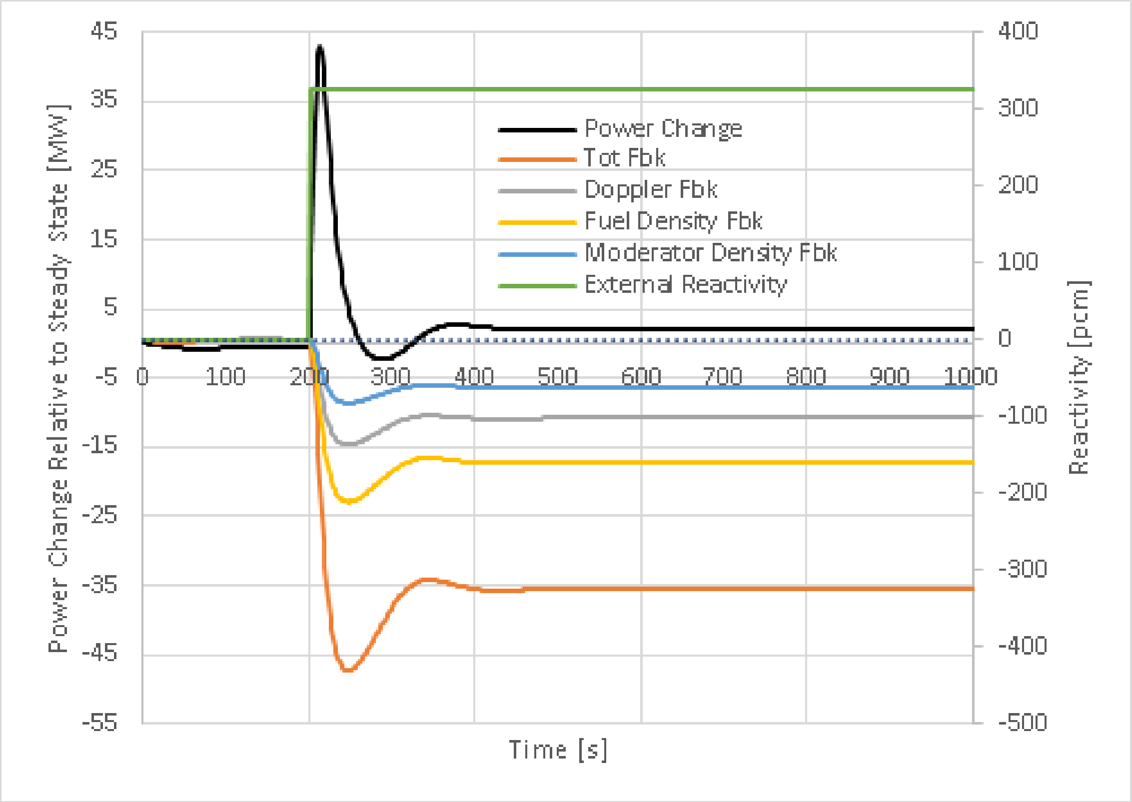
DNP grouping helps with analyses (group decay, abundance

Process of DNP advection with flowing fuel is DNP "drift"

Cannot neglect the kinetic/dynamic implications of DNP "drift



FFPRKEs - Standard Point Reactor Kinetics Equations



By way of reminder…Textbook 6 DNP group PRKE's

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

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

DNP drift

- Leads to lower effective DN fraction,
- Looks like a negative reactivity insertion, and
- Introduces a "reactivity bias" barrier to criticality for a given flow

Relatively lower DN emission in core as core DNP inventory decreases

Relatively higher DN emission in core as core DNP inventory increases

Fuel flow (e.g. as driven by fuel pump) has direct reactivity implications

FFPRKEs – Formulation

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

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

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

$$\bar{\beta} = \beta - \left(\frac{\Lambda}{P(t)}\right) \sum_{i=1}^{6} \lambda_i C_i^L(t)$$

A - In-Vessel DNP gain by fission
B - In-Vessel DNP loss by decay, flow
C - In-Vessel DNP gain by Ex-Vessel DNP flow
D - Ex-Vessel DNP gain by In-Vessel DNP flow
E - Ex-Vessel DNP loss by decay, flow

Where:

$P(t)$= Thermal power due to fission 0

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

C_i^L= delayed neutron precursor group i inventory/concentration ex-core

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

FFPRKEs – Steady State Initialization

Assume:

- Criticality at some power
- Steady flow (time derivatives of dependent variables ze
- No feedback or control reactivity

Given initial power P_0, derive initial values for:

- All DNP variables by cohort
- Bias reactivity
- Effective DN fraction

These are initial conditions for FFPRKE model

Under these assumptions, the steady form of the FFPRK equations is:

$$\frac{dP(0)}{dt} = 0 = \left(\frac{\Delta\rho_0 - \bar{\beta}(0)}{\Lambda}\right) P_0 + \sum_{i=1}^{6} \lambda_i C_{i,0}^{C} = \left(\frac{\Delta\rho_0 - \beta + \beta_{lost}(0)}{\Lambda}\right) P_0 + \sum_{i=1}^{6} \lambda_i C_{i,0}^{C}$$

$$\frac{dC_i^C(0)}{dt} = 0 = \left(\frac{\beta_i}{\Lambda}\right) P_0 - \left(\lambda_i + {}^{2}/_{\tau_C}\right) C_{i,0}^{C} + \left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^{2}/_{\tau_L}\right) C_{i,0}^{L}, \qquad i = 1 \ldots 6$$

$$\frac{dC_i^L(0)}{dt} = 0 = \left(\frac{V_C}{\tau_C V_L}\right) C_{i,0}^{C} - \left(\lambda_i + {}^{1}/_{\tau_L}\right) C_{i,0}^{L}, \qquad i = 1 \ldots 6$$

Solving for DNP cohorts:

$$C_{i,0}^{C} = \alpha_i P_0, \qquad i = 1 \ldots 6$$

$$C_{i,0}^{L} = \gamma_i \alpha_i P_0 = \gamma_i C_{i,0}^{C}, \qquad i = 1 \ldots 6$$

$$\gamma_i = \left(\frac{V_C}{\tau_C V_L}\right) \Big/ \left(\lambda_i + {}^{1}/_{\tau_L}\right), \qquad i = 1 \ldots 6$$

$$\alpha_i = \left(\frac{\beta_i}{\Lambda}\right) \Big/ \left[\left(\lambda_i + {}^{2}/_{\tau_C}\right) - \gamma_i \left(\left(\frac{V_L}{V_C}\right)\left(\lambda_i + {}^{2}/_{\tau_L}\right)\right)\right], \qquad i = 1 \ldots 6$$

Solving for the bias reactivity and the time-zero effective delayed neutron fraction:

$$\Delta\rho_0 = \beta - \Lambda \sum_{i=1}^{6} \lambda_i \alpha_i (1 + \gamma_i)$$

$$\bar{\beta}(0) = \beta - \beta_{lost}(0) = \beta - \Lambda \sum_{i=1}^{6} \lambda_i \gamma_i \alpha_i$$

FFPRKEs – “Perfect” Control System Model

Given the set of FFPRK equations and assuming some arbitrary change in fuel flow, an equation can be derived for the time-dependent reactivity intervention of a “perfect control system” that counteracts flow reactivity effects and preserves system criticality. Initially, the reactor is critical with some bias reactivity $\Delta\rho_0$ at some power P_0 with some fuel flow characterized by fluid volumes and core/loop transit times. Assuming the time derivative of reactor power stays at zero and substituting the static and lost delayed neutron fractions for the effective delayed neutron fraction:

$$\left(\frac{\Lambda}{P_0}\right)\frac{dP(t)}{dt} = 0 = \Delta\rho_0 + \rho_{fb}(t) + \rho_{cr}(t) - \beta + \left(\frac{\Lambda}{P_0}\right)\sum_{i=1}^{6}\lambda_i\left(C_i^C(t) + C_i^L(t)\right) \tag{20}$$

Then, solving for the value of $\rho_{cr}(t)$ assuming no feedback reactivity:

$$\rho_{cr}(t) = \left(\frac{\Lambda}{P_0}\right)\left(\sum_{i=1}^{6}\lambda_i\left(\left(C_{i,0}^C - C_i^C(t)\right) + \left(C_{i,0}^L - C_i^L(t)\right)\right)\right) \tag{21}$$

As time goes on and as the FFPRK model is being solved, an external control reactivity following this prescription will hold reactor power approximately constant despite DNP drift due to flow changes. The situation is more complicated if temperature feedback is involved, but for a zero-power flow reactivity transient this result proves particularly useful.

FFPRKEs – Auxiliary Quantities

Gross characteristics of core and loop flow are used in equation source/sink terms to describe DNP drift

- Transit times approximate the time required for flow to traverse both the active core and the balance of the primary loop
- F… ulated from CV's that comprise the core and loop

$$V_C = \sum_{j=1}^{N_C} V_j$$

"core" quantities consider all CV's identified as belonging to the core

$$V_L = \sum_{j=1}^{N_L} V_j$$

"loop" quantities consider all CV's identified as belonging to the balance of the loop

$$\tau_C = \frac{1}{V_C} \sum_{j=1}^{N_C} (vAV)_j$$

Resort to control volume averaged notions of flow path phasic (pool) flows

$$\tau_L = \frac{1}{V_L} \sum_{j=1}^{N_L} (vAV)_j$$

MELCOR MSR
Modeling and Development
Thermal Hydraulics – Practice

Input Structures – FLiBe EOS

Global input record READFLUID declares alternate EOS

- Fluid files contain information required to “replace” the default condensable hydrodynamic material (water)
- Fluid files distributed with MELCOR executables
- FLiBe defined by property file named ‘tpffi’
  - Name the fluid file in MELCOR global input
  - Ensure the fluid file is located in the same directory as the input file to run

```
Input file: msre.inp
meg_diagfile      'msreg.dia'
meg_outputfile    'msreg.out'
meg_restartfile   'msre.rst'
mel_diagfile      'msre.dia'
mel_outputfile    'msre.out'
extdiagf          'msre.ext'
mel_restartfile   'msre.rst' ncycle 0
plotfile          'msre.ptf'
messagefile       'msre.mes'
fluidfile         'tpffi'
defaultdirectory   '.\output'
```

Corollary: CVH_SUPERCOOLPOOL and “freezing”

- Special treatment internal to EOS related to internal energy calculat
- Cope with the approach to hydrodynamic material freezing (e.g. salt spill scenario)
- Hydrodynamic pool not allowed to form a solid phase in CV per se, but upon “freezing” hold as a supercooled pool
- Supercooling:
  - Pool cools to below its freezing point in a nonequilibrium condition temporarily precluding solid phase formation
  - Supercooled liquid “waits” on homogeneous nucleation for a reversion from nonequilibrium
- Check for potentially problematic internal energy predictions from EOS under these conditions
- Adjust internal energy predictions and allow calculation to proceed
- Best practice – use CVH_SUPERCOOLPOOL in MSRs generally or at least when salt freezing is a possibility

Input Structures – CVH Fluid Core

CVH Record	Description
CV_FLUIDFUEL	Identify the "core" CV type and the "loop" CV type
CV_FISPOWDIST	Specify a reactor power spatial shape distribution across all "core" CVs

```
cv_fluidfuel              'Vessel'     'Loop'        ! Core CVs are of type 'Vessel' and Loop CVs are of type 'Loop' from CV_TYP control volume block input
cv_fispowdist 'Core_fPow'    1.000000       10           5            ! CF 'Core_fPow' furnishes power level/magnitude, 10 CVs of type 'Vessel' comprise core
                                                                      ! 10 CVs of type 'Vessel' comprise core, 5 CVs of type 'Loop' comprise balance of primary
        1          'CoreCV1'     0.000000    0.0  0.0  0.0  0.0      ! Note table should be 10 rows long (1 entry per CV in core)
…
        10         'CoreCV10'    0.002107    1.0  0.0  0.0  0.0      !  N NameCV ZFAC RFAC … final 3 real type variables are defunct inputs
```

Above defines a 10 CV active core and a 5 CV balance-of-primary as the full primary fuel flow loop

- CF-specified power magnitude P_0
- CoreCV1 has no power (zero for ZFAC and/or RFAC)
- CoreCV10 has a fission power generation rate equal to ZFAC*RFAC*P_0

CV_FLUIDFUEL also serves as an activation record for fluid fuel modeling capabilities

Input Structures – FFPRKEs

CVH Record	Description
CV_FLUIDFUELPKM01	Specify FFPKM start time and initial steady power
CV_FLUIDFUELPKM02	Specify external reactivity and any external neutron source
CV_FLUIDFUELPKM03	Configure reactivity feedback options

```
cv_fluidfuelpkm01    -100.0    1000000.0    ! Turn on FFPRKE model at -100.0 s problem time ; Initial power set
cv_fluidfuelpkm02    'React'   'Zero'       ! CF 'React' specifies an external reactivity component, and CF 'Zero' defines an external neutron source
cv_fluidfuelpkm03    0                      ! Integer flag of 0 declares that no reactivity feedbacks should be computed internally by MELCOR
```

Above record format is similar to analogous COR_PKMXX for standard fixed fuel PRKEs

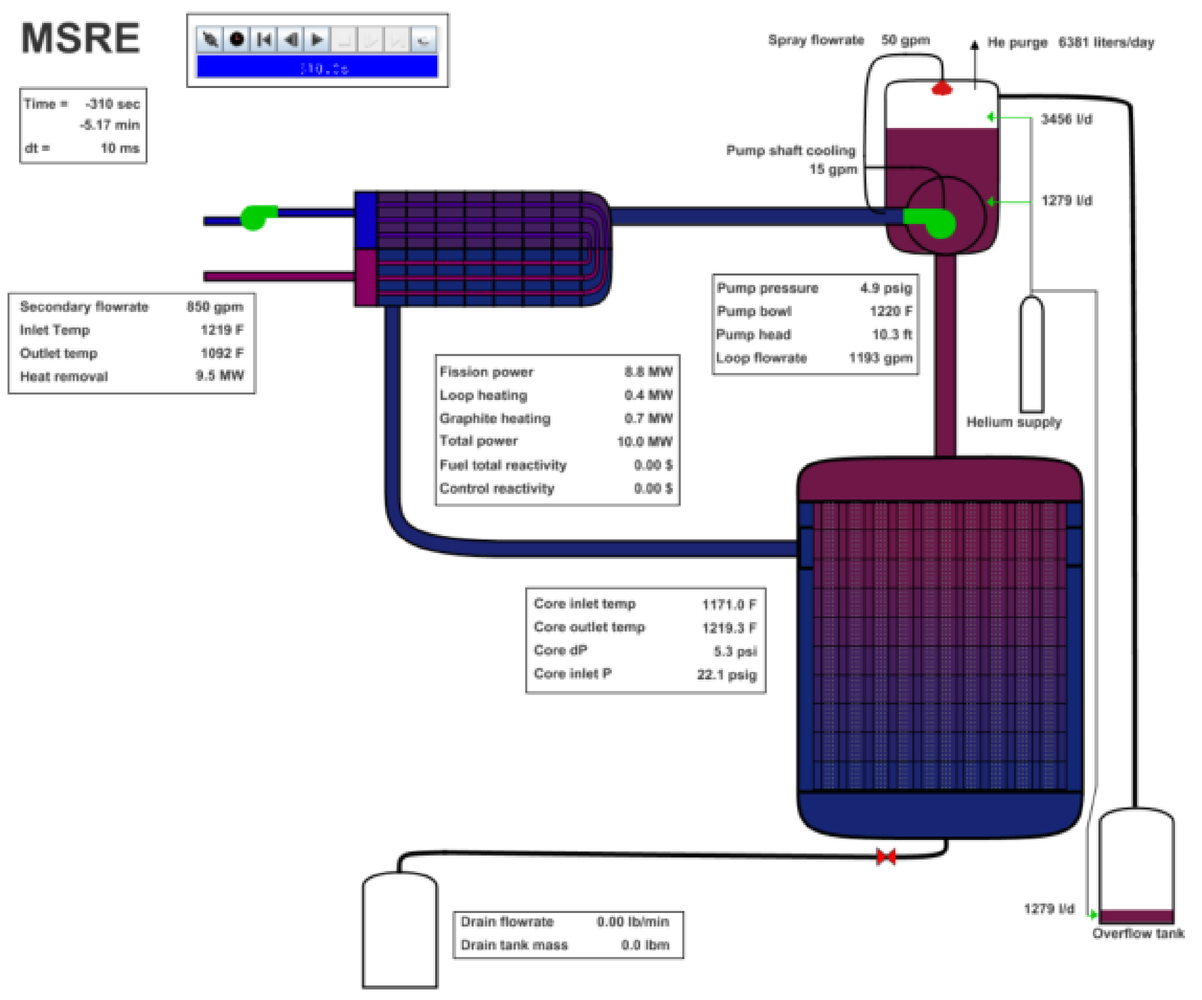
CV_FLUIDFUELPKM01 TSTART QINIT

CV_FLUIDFUELPKM02 NAMECF_REACTIVITY NAMECF_NSOURCE

- NAMECF_REACTIVITY and NAMECF_SOURCE can be 'NO', and NAMECF_SOURCE is optional
- Keyword 'HOLDSTEADY' for NAMECF_REACTIVITY invokes the "perfect control system" model for now

CV_FLUIDFUELPKM03 limited in functionality for now

Example : Zero-Power Flow Coast-Down on Simplified ORNL MSRE




```
CV_FLUIDFUEL 'Vessel' 'Loop'  ! identify "in-vessel" CV type and "loop" CV type
!
CV_FISPOWDIST 'CORPOW' 1.0 12 22 ! CF 'CORPOW' for steady power
   1  'Distrib_100'  0.0000 0.0  0.0 0.0 0.0 ! no power
   2  'Annulus_105'  0.0000 0.0  0.0 0.0 0.0 ! no power
   3  'Core_Inlet'   0.0000 0.0  0.0 0.0 0.0 ! no power
   4  'Core_111'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   5  'Core_112'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   6  'Core_113'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   7  'Core_114'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   8  'Core_115'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   9  'Core_116'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   10 'Core_117'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   11 'Core_118'     0.1250 1.0  0.0 0.0 0.0 ! 1/8
   12 'Core_Out'     0.0000 0.0  0.0 0.0 0.0 ! no power
!
CV_FLUIDFUELPKM01 200.0 10.0       ! start FFPKM at 200.0 s , initial power 10.0 W
CV_FLUIDFUELPKM02 HOLDSTEADY  ! "perfect" control system holds critical
CV_FLUIDFUELPKM03 0                ! disallows temperature feedback ("zero power")
!
```

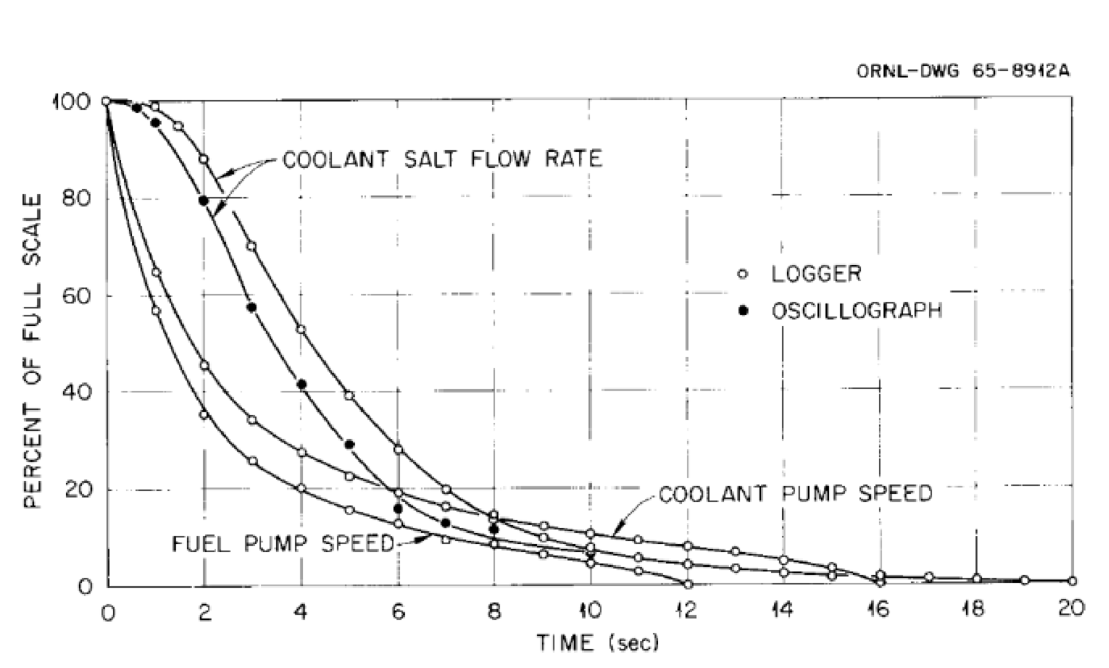
Example : Zero-Power Flow Coast-Down on Simplified ORNL MSRE

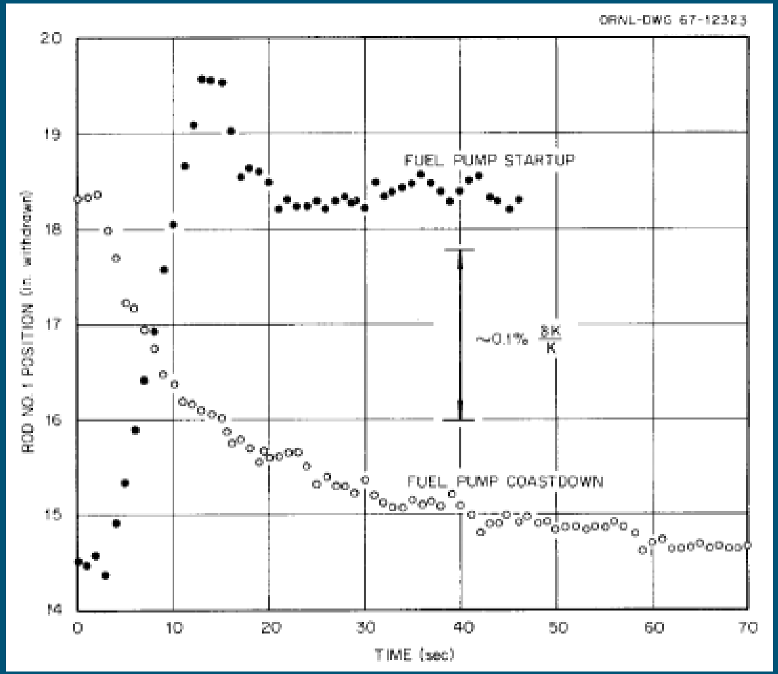
Null transient was checked

- Steady-state MSRE model built, FFPRKE’s start governing power at some problem time given initial power
- Verify steady power level (zero reactivity) and a bias reactivity consistent with experimental value
- Good test of input structures, data read/write, output plots, etc.

Zero-power fuel pump coast-down

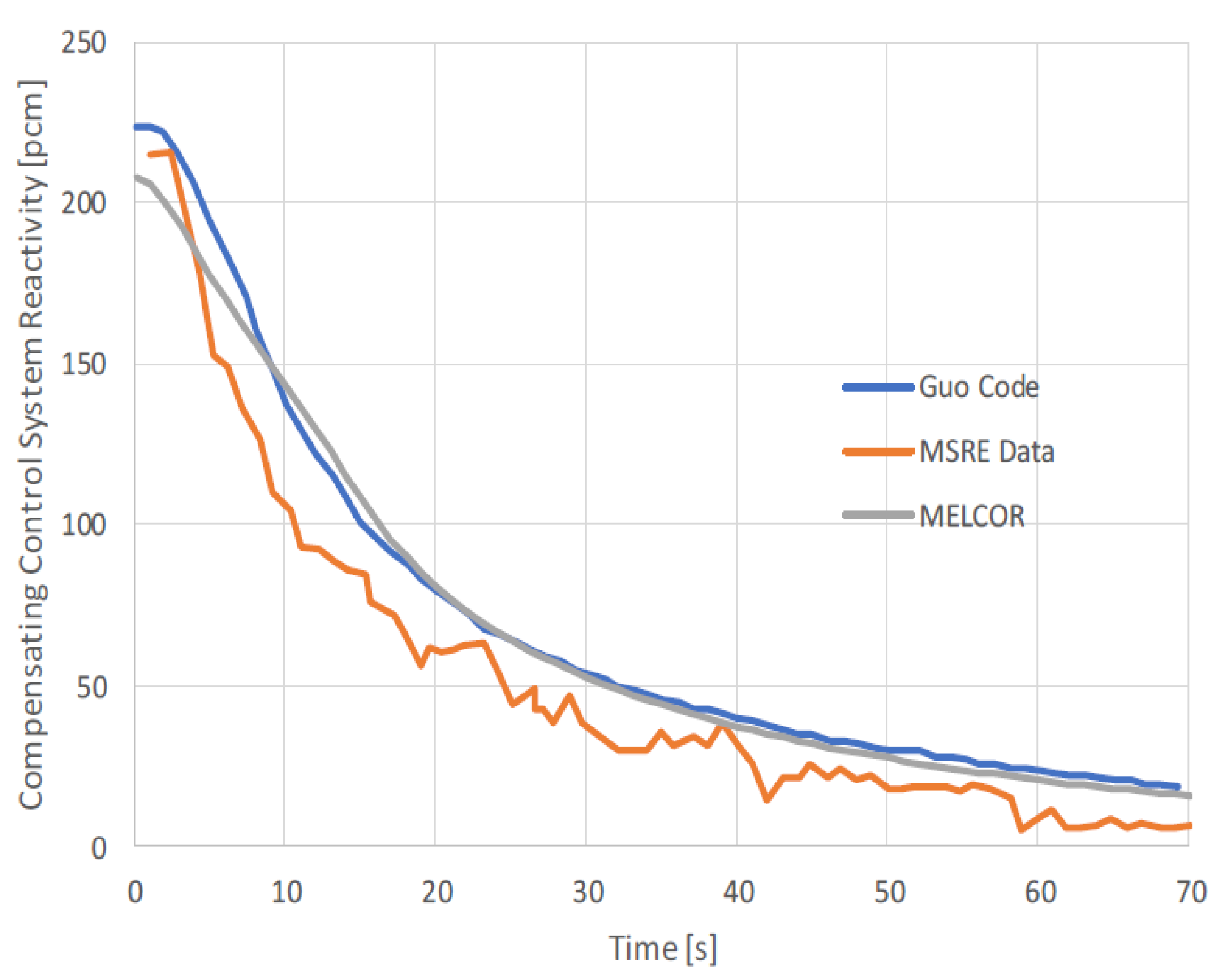
*Fuel circulation worth:
0.212 +/- 0.004 δK/K

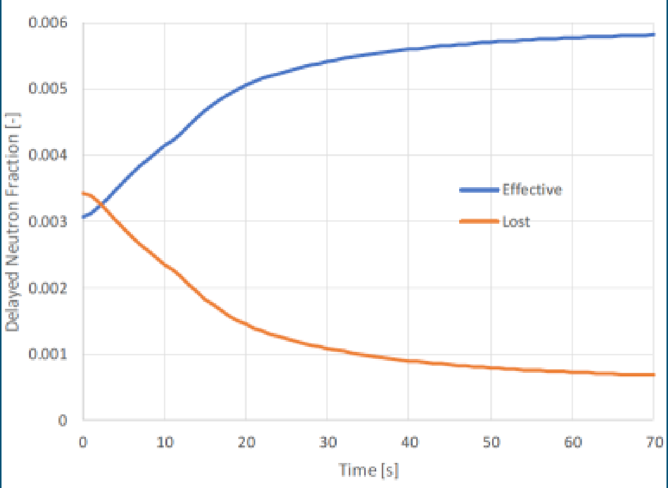


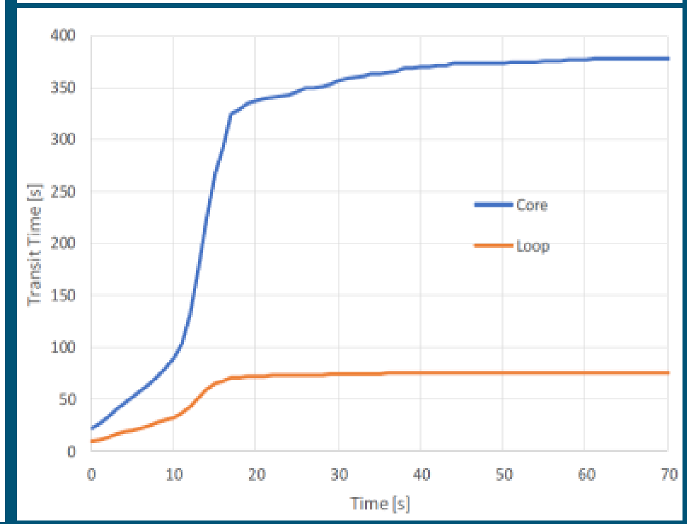


Example : Zero-Power Flow Coast-Down on Simplified ORNL MSRE

Validation of FFPRKE predictions against experimental data and a separate computer code

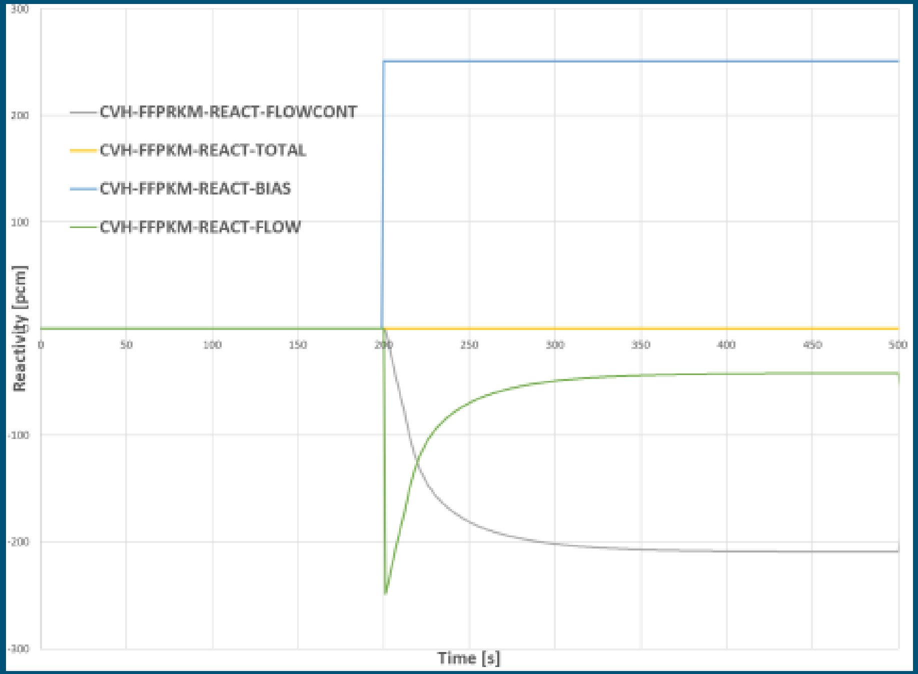






ORNL MSRE Zero-Power Flow Coast-Down Experimental Benchmark

Plot Variable	Description
CVH-FFPKM-POW	Power [W]
CVH-FFPKM-REACT-FEEDBACK	Internally-computed feedback reactivity [pcm]
CVH-FFPKM-REACT-TOTAL	Total balance of reactivity [pcm]
CVH-FFPKM-REACT-BIAS	Bias reactivity [pcm]
CVH-FFPKM-REACT-FLOW	Flow reactivity [pcm]
CVH-FFPKM-REACT-FLOWCONT	External control reactivity of perfect control system model [pcm]
CVH-FFPKM-REACT-CONTROL	External CF reactivity [pcm]
CVH-FFPKM-CORTRANS	Core transit time [s]
CVH-FFPKM-LOOPTRANs	Loop transit time [s]
CVH-FFPKM-LOOPVOL	Loop fluid volume [m^3]
CVH-FFPKM-CORVOL	Core fluid volume [m^3]
CVH-FFPKM-BETAEFF	Effective delayed neutron fraction [-]
CVH-FFPKM-BETALOST	Lost delayed neutron fraction [-]



Conclusions

Thermal hydraulics aspects of MSR modeling in MELCOR were discussed

New input structures were reviewed

Limited validation was performed against experimental data from ORNL MSRE