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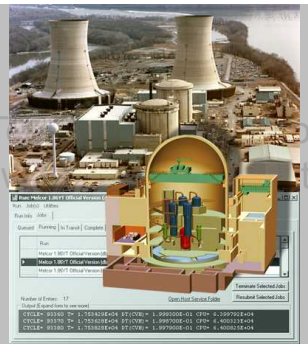

MELCOR/CONTAIN LMR Implementation – Progress FY16

Larry Humphries and David Louie

November, 2016

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Work Scope

- Project Motivation and Objective
  - Address the regulatory infrastructures requirements regarding accident analyses for reactor systems,
    - A sodium coolant accident analysis code is necessary to provide regulators with a means to perform confirmatory analyses for future sodium reactor submissions.
- Solution Strategy
  - Implementation of sodium phenomenology models into an integrated, full-featured, actively maintained, severe accident code
    - CONTAIN-LMR models implemented into the CONTAIN2 code
    - CONTAIN-LMR models implemented into the MELCOR code
    - MELCOR is a mature integrated severe accident code
      - Used by NRC for level 2 and level 3 PRA analysis for LWR as well as
      - Used for containment DBA analysis
      - 30 years of development
      - MELCOR SQA Program
    - New modeling added to MELCOR will be enabled only when sodium models are specified by user, and will not impact code performance.

MELCOR Background

- MELCOR is developed by:
  - US Nuclear Regulatory Commission
  - Division of Systems Analysis and Regulatory Effectiveness
  - Office of Nuclear Regulatory Research
- MELCOR Development is also strongly influenced by the participation of many International Partners through the US NRC Cooperative Severe Accident Research Program (CSARP)
  - Development Contributions – New models
  - Development Recommendations
  - Validation

Software Quality Assurance

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- Sandia Corporate Process Requirement 001.3.6 (CPR 001.3.6)
- The software management framework adapted from two internationally recognized standards
  - Capability Maturity Model Integration (CMMI) ®
  - ISO 9001
- US NRC SQA requirements
  - NUREG/BR-0167
- These standards provide elements of traceability, repeatability, visibility, accountability, roles and responsibilities, and objective evaluation

MELCOR Software Quality Assurance Best Practices

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Emphasis is on Automation

Affordable solution

Consistent solution

- MELCOR Wiki
  - Archiving information
  - Sharing resources (policies, conventions, information, progress) among the development team.
- Code Configuration Management (CM)
  - 'Subversion'
  - TortoiseSVN
  - VisualSVN integrates with Visual Studio (IDE)
- Code Review
  - Code Collaborator
- Nightly builds & testing
  - DEF application used to launch multiple jobs and collect results
  - HTML report
  - Regression test report
- Regression testing and reporting
  - More thorough testing for code release
  - Target bug fixes and new models for testing
- Bug tracking and reporting
  - Bugzilla online
- Validation and Assessment calculations
- Documentation
  - Available on Subversion repository with links from wiki
  - Latest PDF with bookmarks automatically generated from word documents under Subversion control
    - Links on MELCOR wiki
- Sharing of information with users
  - External web page
  - MELCOR workshops
  - Possible user wiki

MELCOR/CONTAIN-LMR Implementation

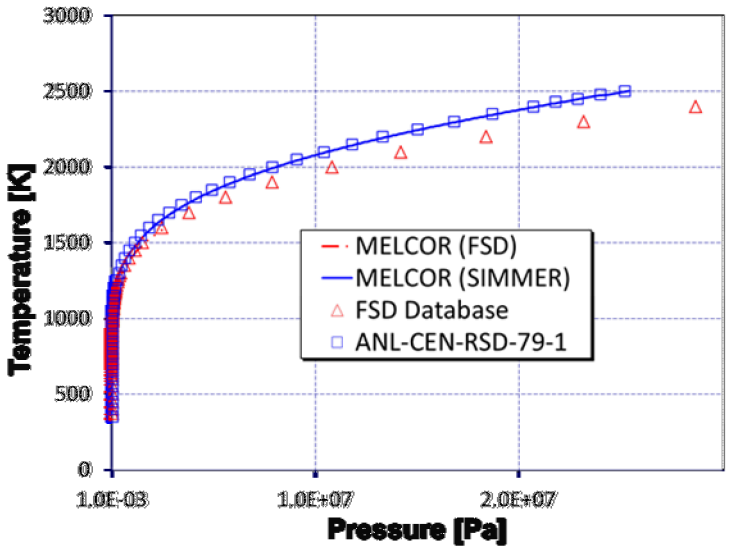
- Phase 1 – Implement sodium as replacement to the working fluid for a MELCOR calculation
  - Implement properties & Equations Of State (EOS) from the fusion safety database
  - Implement properties & EOS based on SIMMER-III
- Phase 2 – Review of CONTAIN-LMR and preparation of design documents
  - Detailed examination of LMR models with regards to implementation into MELCOR architecture
  - Updating CONTAIN-LMR and CONTAIN2 to MELCOR development standard
- Phase 3 – Implementation and Validation of:
  - Implementation of CONTAIN/LMR models into CONTAIN2
  - Sodium spray fires (ongoing)
  - Atmospheric chemistry (ongoing)
  - Sodium pool chemistry (ongoing)
- Phase 4 – Implementation and Validation of:
  - Condensation of sodium
  - Sodium-concrete interactions (SLAM model)
  - Debris bed/concrete cavity interactions (no interest from DOE)

CONTAIN2-LMR Development

- CONTAIN2 is last version of CONTAIN development
  - Significant improvements over CONTAIN-LMR
  - CONTAIN-LMR only works for sodium problems
  - Available standard test sets for LWR applications
- Development of CONTAIN2-LMR
  - Port all sodium models from CONTAIN-LMR
  - Allows to run both LWR and sodium reactor problems
- Verification – same sets as in CONTAIN-LMR
  - Two condensable option and atmospheric chemistry model test problems
  - Experiments for pool and spray fires – AB1, AB5
  - Sandia SLAM experiments for sodium-concrete interactions

Sodium Coolant in MELCOR 2.1

- Sodium Working fluid
  - Implement Sodium Equations of State (EOS)
  - Implement Sodium thermal-mechanical properties
- Two models implemented
  - Fusion safety database (FSD)
  - SIMMER database (SASA 4)
- Sodium properties for FSD are mainly read from an input file, so it is easy to adapt for other liquid metal fluids
- Test problems have been created demonstrating model capability
- Some improvement, particularly for FSD, may require additional assessment and development



Spray Fire Chemistry

- Based on NACOM spray model from BNL
  - Input requirement: fall height, mean diameter and source
  - Internal droplet size distribution (11 bins) from Nukiyama-Tanasama correlation
  - Reactions considered:
    - (S1) $2\ \mathrm{Na} + {}^{1}/_{2}\,\mathrm{O_2} \rightarrow \mathrm{Na_2O}$,
    - (S2) $2\ \mathrm{Na} + \mathrm{O_2} \rightarrow \mathrm{Na_2O_2}$
  - Fixed ratio of peroxide and monoxide $\left(\frac{1.3478 \cdot \mathrm{F}_{Na_2O_2}}{1.6957 - 0.3479 \cdot \mathrm{F}_{Na_2O_2}}\right)$
  - CONTAIN Routine Ported to MELCOR: SPRAY
  - Tracked quantities include:
    - Mass of Na (spray, burned, pool), O_2(consumed), Na_2O_2+ Na_2O(produced)
    - Energy of reactions

Pool Fire Chemistry

- Based on SOFIRE II code from ANL
  - Reactions considered:
    - (P1) $2\,\mathrm{Na} + \mathrm{O_2} \rightarrow \mathrm{Na_2O_2}$,
    - (P2) $4\,\mathrm{Na} + \mathrm{O_2} \rightarrow 2\,\mathrm{Na_2O}$
  - Reactions depend on the oxygen diffusion as: $\mathrm{D} = \frac{6.4315\times10^{-5}}{\mathrm{P}}\mathrm{T}^{1.823}$
  - Input requirement:
    - F1 – fraction of O_2 consumed for monoxide, F2 – fraction of reaction heat to pool, F3 – fraction of peroxide mass to pool, & F4 – fraction of monoxide mass to pool
  - PFIRE routine will be ported to MELCOR 2.1
- Tracked quantities:
  - Mass of Na(pool, burned), O_2(consumed), Na_2O_2+Na_2O(produced)
  - Energy of reactions

Atmospheric Chemistry

- A number of reactions have been considered:
  - (A1) $\mathrm{Na(l) + H_2O\ (l) \rightarrow NaOH(a) + \frac{1}{2}H_2}$
  - (A2) $\mathrm{2\ Na(g,l) + H_2O\ (g,l) \rightarrow Na_2O(a) + H_2}$
  - (A3) $\mathrm{2\ Na(g,l,a) + \frac{1}{2}O_2\ or\ O_2 \rightarrow Na_2O(a)\ or\ Na_2O_2(a)}$
  - (A4) $\mathrm{Na_2O_2(a) + 2\ Na(g,l) \rightarrow 2\ Na_2O(a)}$
  - (A5)
    - $\mathrm{Na_2O(a) + H_2O\ (g,l) \rightarrow 2NaOH(a)}$
    - $\mathrm{Na_2O_2(a) + H_2O\ (g,l) \rightarrow 2NaOH(a) + 0.5O_2}$
- All these reactions are assumed to occur:
  - Atmosphere (g), aerosol, surfaces (i.e., HS)
  - The order of the reactions are given

Atmospheric Chemistry (concluded)

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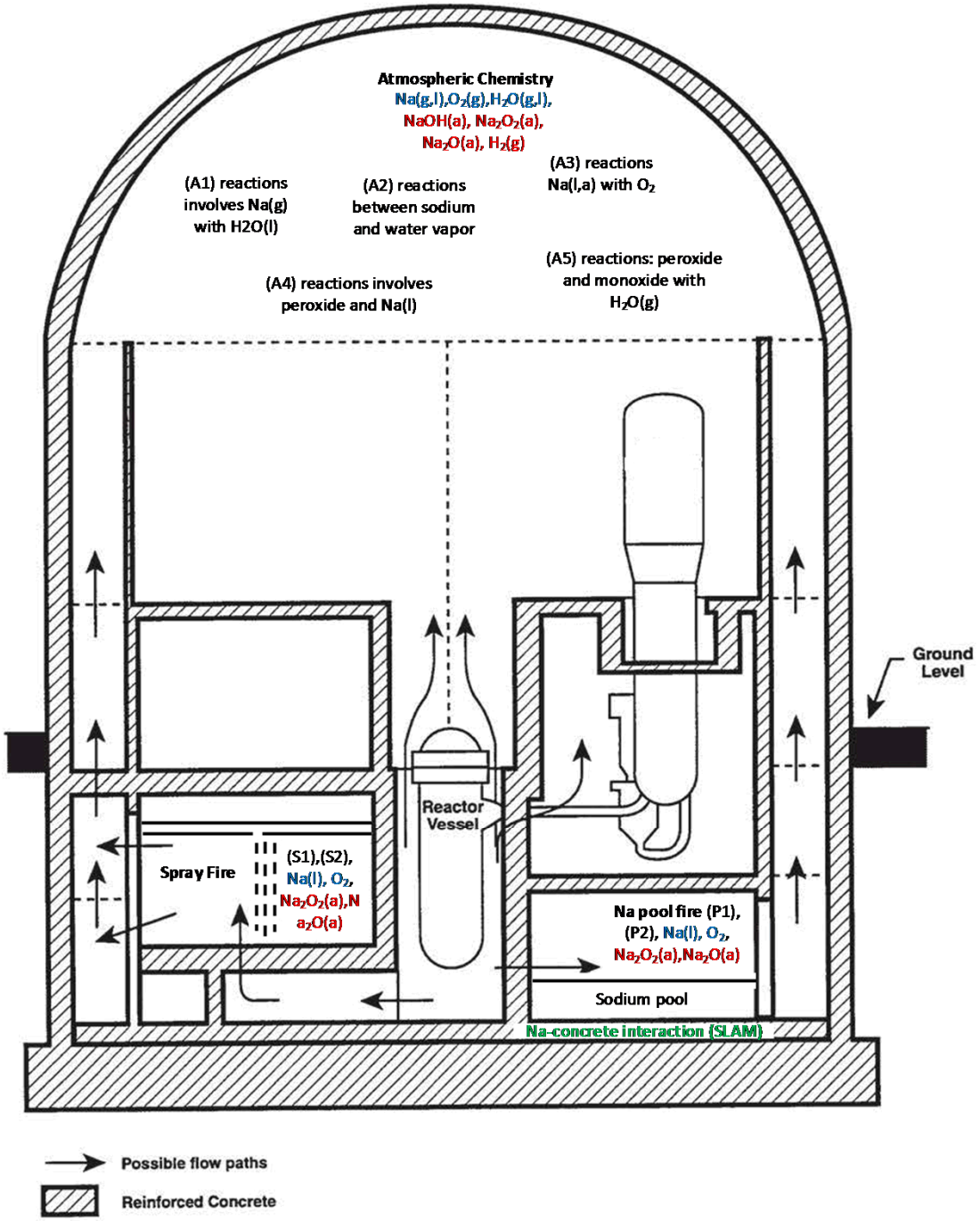
- Porting routines:
  - CHEMRX - main driven routine to call:
    - CHMGAS – gas-to-gas reactions
    - CHMAER – aerosol-to-gas reactions
    - CHMDEP – deposited aerosol reactions
    - CHMREP – aerosol-to-liquid reactions on surfaces
  - Interface variables – RN, CVH, NCG, BUR packages
- Outputs
  - Reaction number, reaction energy, byproducts (Na classes, H_2), gas and liquid consumed (Na, H_2O, O_2)


Atmospheric Chemistry
Na(g,l),O2(g),H2O(g,l),
NaOH(a), Na2O2(a),
Na2O(a), H2(g)
(A1) reactions involves Na(g) with H2O(l)
(A2) reactions between sodium and water vapor
(A3) reactions Na(l,a) with O2
(A4) reactions involves peroxide and Na(l)
(A5) reactions: peroxide and monoxide with H2O(g)
Ground Level
Reactor Vessel
Spray Fire
(S1),(S2), Na(l), O2, Na2O2(a),Na2O(a)
Na pool fire (P1), (P2), Na(l), O2, Na2O2(a),Na2O(a)
Sodium pool
Na-concrete interaction (SLAM)
Possible flow paths
Reinforced Concrete

Sodium Chemistry (NAC) Package Development

- To better manage the sodium related chemistry models
- NAC Package
  - Data structures – in module (M_NAC)
    - NaCL(5), old-new variables, input parameters
  - RN to NAC class structure – tracks aerosol products
  - Na modeled as condensable, H2O modeled as aerosol
  - Sensitivity coefficient development (a minimum set for now)
  - Interface variables, interface with many packages, for examples:
    - NCG – O_2 and H_2
    - HS – condensate, deposits
    - CVH – Na, reaction energies
    - RN – aerosol interactions: Na, H2O, NaOH, Na2O, Na2O2
  - Calling sequence for NAC model executions

NAC Package Subroutines

- M_NAC – data structure module and specialized subroutines for data processing and supporting various chemistry model routines
- NAC_GENERATEDB – Subroutine for the MELGEN
- NAC_NACDBD –Executive level routine to call NACRUN
- NAC_NACRUN – High level subroutine to run various chemistry models
- NAC_PFIRE – Pool fire run routine
- NAC_RW – MELGEN input processing for all NAC MELGEN inputs, and restarts
- NAC_SPRAY – Spray fire run routine
- NAC_CHEMRX – Atmospheric chemistry (AC) main routine, which calls NAC_CHMAER, NAC_CHMDEP, NAC_CHMGAS, and NAC_CHMREP. Not completely implemented yet
- NAC_CHMAER –aerosol chemistry routine
- NAC_CHMDEP – deposited chemistry routine
- NAC_CHMGAS – Gas chemistry routine
- NAC_CHMREP – Repository chemistry routine
- NAC_EDIT – Editing routine for NAC models. Currently only spray fire and pool fire outputs are provided

Specified Details on NAC Package

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- New MELGEN records (mostly complete)
  - NAC_INPUT
  - NAC_RNCLASS
  - NAC_ATMCHEM
  - NAC_SPRAY
  - NAC_PFIRE
  - NAC_COND
  - NAC_SLAM (not yet)
  - NAC_SC (not yet)
  - BUR_NAI
- Plot and control function variables (not yet)
- Outputs (not yet)

MELCOR Default RN Class Structure

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Class	Class Name	Chemical Group	Represent	Member Elements
1	XE	Noble Gas	Xe	He, Ne, Ar, Kr, Xe, Rn, H, N
2	CS	Alkali Metals	Cs	Li, Na, K, Rb, Cs, Fr, Cu
3	BA	Alkaline Earths	Ba	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	I2	Halogens	I_2	F, Cl, Br, I, At
5	TE	Chalcogens	Te	O, S, Se, Te, Po
6	RU	Platinoids	Ru	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	MO	Early Transition Elements	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8	CE	Tetravalent	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	LA	Trivalents	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
10	UO2	Uranium	UO_2	U
11	CD	More Volatile Main Group	Cd	Cd, Hg, Zn, As, Sb, Pb, Tl, Bi
12	AG	Less Volatile Main Group	Ag	Ga, Ge, In, Sn, Ag
13	BO2	Boron	BO_2	B, Si, P
14	H2O	Water (working fluid)	H_2O	H_2O
15	CON	Concrete	CON	- – -
16	CSI	Cesium iodide	CsI	CsI
17	CSM	Cesium Molybdate	CsM^1	CsM^1

RN Class to NAC Mapping

NAC_RNCLASS – Aerosol mapping
Optional
This record is required to map classes from the RN package to NAC package. Note that when sodium is the working fluid, class 14 becomes sodium and all SCs map to sodium. Thus the user is required to define the water aerosol class as "H2Oa" for modeling any water reactions, since water in sodium reactor analyses is being treated as a trace material. Thus SC7110 may be modified for water in the new RN class. Similarly, the molecular weight may be input. Only five input variables are required.

(1) RN class number for water. No default
(type = integer, default = none, units = dimensionless)
(2) RN class number for sodium. Default=14 (see Table x)
(type = integer, default = 14, units = dimensionless)
(3) RN class number for NaOH. No default.
(type = integer, default = none, units = dimensionless)
RN class number for Na2O2. No default
(type = integer, default = none, units = dimensionless)
(5) RN class number for Na2O. No default
(type = integer, default = none, units = dimensionless)

Sodium Atmosphere Chemistry Input

NAC_ATMCHEM – Sodium Atmosphere Chemistry Model

Optional

This model allows the modeling of the atmosphere chemistry in a given control volume if the sodium is present in the atmosphere.

(1) NUM - The number of control volumes to include this model

(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC Table row index.

(type = integer, default = none, units = none)

(2) CVHNAME

The name of the CVH volume.

(type = character, default = none, units = dimensionless)

(3) FRNA2O

The fraction of sodium that produces Na2O versus Na2O2 with oxygen (Eq. 1-3).

(type = real, default = 0.5, units = dimensionless)

Sodium Spray Fire Model

NAC_SPRAY – Sodium Spray Fire Model

Optional

This model enables the modeling of the sodium spray fire in a given control volume if the sodium spray source is given.

(1) NUM The number of control volumes to include this model
(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC Table row index.
(type = integer, default = none, units = none)

(2) CVHNAME The name of the CVH volume.
(type = character, default = none, units = none)

(3) HITE Fall height of sodium spray. Default is CVH height.
(type = real, default = CVH volume height, units = m)

(4) DME Mean sodium droplet diameter.
(type = real, default = 0.001, units = m)

(5) FNA2O2 Fraction of sodium peroxide produced by the spray fire.
(type = real, default = 1.0, units = m)

(6) SOU-TYPE Sodium spray source type: TF or CF. Default is TF. Note that two tables are expected: mass and temperature/enthalpy
(type = character, default = TF, units = none)

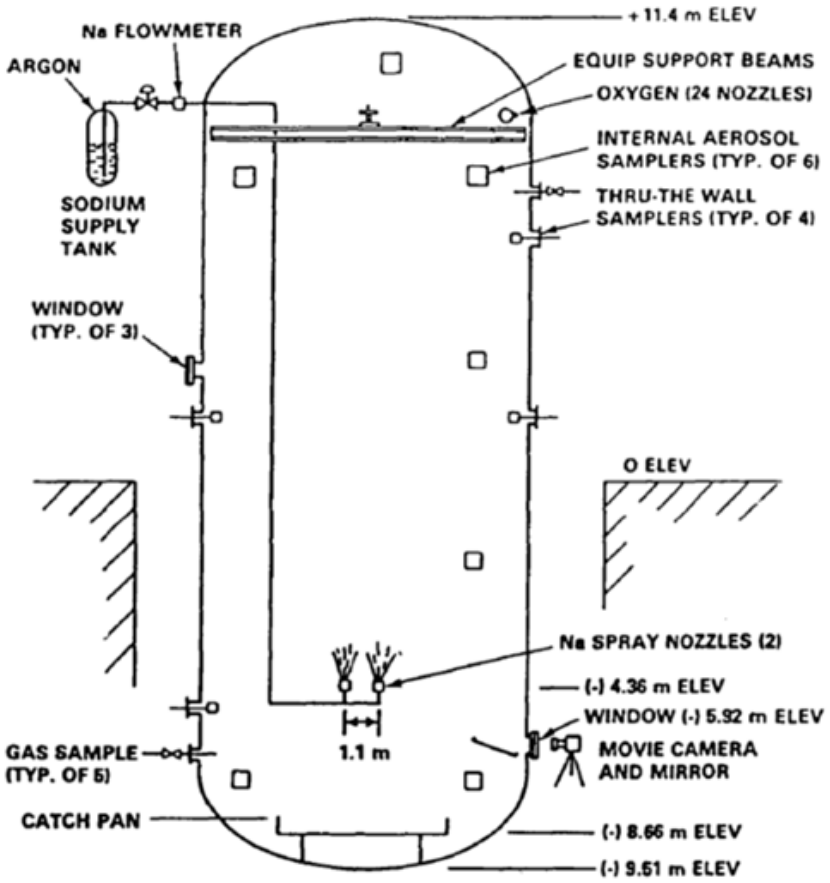
(7) MASS-NAME Name of the TF or CF for the mass source.
(type = character, default = none, units = kg/s)

(8) THERM-NAME Name of the TF or CF for the temperature of the source.
(type = character, default = none, units = temperature)

Sodium Spray Fire -Verification and Validation Tests

The ABCOVE test (AB-5)

- was to provide experimental data for validating aerosol behavior of the computer codes during a sodium spray fire scenario. 223 kg of sodium was injected into a 852 m^3 of the vessel.
  - Experimental results showed aerosol generated (60% Na_2O_2 and 40% NaOH)
- CONTAIN model –
  - A single cell is used for this vessel
  - Walls, roof and floor HSs are modeled
  - Input value for sodium peroxide fraction is set to 1.0
  - Test condition is being modeled



Sodium Pool Fire

NAC_PFIRE – Sodium Pool Fire Model

Optional

This model allows the modeling of the sodium pool fire in a given control volume. A number of fraction inputs can be specified.

(1) NUM The number of control volumes to include this model

(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC Table row index.

(type = integer, default = none, units = none)

(2) CVHNAME The name of the CVH volume.

(type = character, default = none, units = none)

(3) FO2 Fraction of the oxygen consumed that reacts to form monoxide. 1-FO2 is the remaining oxygen fraction for the reaction to form peroxide.

(type = real, default = 0.5, units = none)

(4) FHEAT Fraction of the sensible heat from the reactions to be added to the pool. The balance will go to the atmosphere.

(type = real, default = 1.0, units = none)

(5) FNA2O Fraction of the Na_2O remaining in the pool. The balance will be applied to the atmosphere as aerosols.

(type = real, default = 1.0, units = none)

(6) FNA2O2 Fraction of the Na_2O_2 remaining in the pool. The balance will be applied to the atmosphere as aerosols.

(type = real, default = 0.0, units = none)

Accomplishments

- Phase I:
  - Enabled and documented the sodium property models in MELCOR 2.1
    - FSD
    - SIMMER
  - Conducted testing for these models
  - Enabled CONTAIN-LMR to be working under MELCOR code development platform
- Phase II:
  - Began implementation of CONTAIN-LMR sodium models into MELCOR 2.1
    - Strategized the implementation method for "Two-condensable Option" and other physics models
    - Validated and verified codes with existing experiments or known results
  - Enabled CONTAIN2 working under MELCOR code development platform and began implementing CONTAIN-LMR sodium models
- Phase III:
  - Re-directed priority of implementation plan due to recent aerosol upgrade in MELCOR 2.1
  - Began to implement sodium chemistry models instead
  - 92% completion on CONTAIN2-LMR
- Phase IV:

Task	Status
CONTAIN2-LMR	Completed
Input processing	Mostly completed (except 2-phase condensable model)
Sodium Spray Fire Model	Fully Implemented and now testing
Sodium Pool Fire Model	Fully Implemented
Sodium Pool Physics Model	Completed
Atmosphere Chemistry Model	Started

Work Scope Breakdown for FY17

- Phase IV –Validation of CONTAIN chemistry and physics models:
  - Development testing – ABCOVE AB5, CSTF AB1
  - Code-to-Code comparison – MELCOR, CONTAIN-LMR and/or CONTAIN2-LMR
  - Implementation of Sodium-concrete interactions (SLAM)
- Final report

JAEA CONTAIN-LMR Updates

- In August 2016, JAEA provided Changes to CONTAIN-LMR Code (CNWG-NE01-RM2-0001, Rev 0)
  - Five subroutines, mainly for Spray Fire Modeling
    - Combustion Energy change:
      - Na_2O from 9.18 to 13.71 MJ/kg of sodium
      - Na_2O_2 from 10.46 to 15.88 MJ/kg of sodium
    - Ability to model spray upward and downward direction with initial velocity input
    - Draft coefficient of spray droplet f(Re)
    - Time step controls for the sodium droplet with O2 in atmosphere

Proposed Sodium Source Term/Safety

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Development Topics	Areas	Notes
Hot Gas Layer	Source Term Safety	During sodium fires, a hot gas layer is formed which causes a rapid temperature gradient in a given room. The reaction rates of sodium aerosols and the transport behavior of aerosols vary with temperature. Thus, accurately modeling the formation of the hot gas behavior is important to reactions and transport behavior of aerosols.
Entrainment of the radionuclides near the surface of the pool fire	Source Term	Contaminated pool fires may require a multi-component model in order to accurately capture the impacts of evaporative entrainment in in the transport of contaminates into the aerosol. Modeling the radionuclides suspended in the sodium aerosols during a sodium pool fire is likely important for accurate source term analysis.
Two Condensable Fluid	Safety	Important for sodium/water interfaces (e.g., steam generators) that are important to support the overall plant safety-case. The sodium found in these interfaces are intentionally non-radioactive in typical SFR designs.
Oxygen Entrainment into a pool fire	Source Term Safety	The oxidation reaction rate of a sodium pool fire is a function of the oxygen available at the pool surface. FUEGO simulations would be utilized to create a reduced order model to capture the flow of oxygen radially along the pool fire surface.
Crust behavior during sodium pool fires	Source Term Safety	During a pool fire, if the sodium pool reaches a saturation limit as a function of temperature of sodium oxide, or other compounds, a crust will form on the pool to limit further reaction between the sodium and oxygen.
Treatment of Isotope Decay	Source Term	Sodium reactor source term analysis may involve aerosols that were held up inside the reactor and/or containment for weeks after the accident initiation. MELCOR will be modified to track radionuclide decay and transition between radionuclide chemical classes.

Backups

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Sodium Spray Fires

- Postulated coolant pipe break or breach of vessel upper head
  - Based on NACOM code
  - Assumed droplet distribution
    - Combustion rate for each droplet size as a function of the fall velocity, the gas and droplet temperatures, the oxygen content in the atmosphere, and the ratio of the mass of oxygen reacted to that of sodium.
- Validate against ABCOVE experiments (i.e., AB-5) – chemistry and aerosol
- Validate against Sandia Sodium fire tests (2011)
  - 2 in-vessel tests
  - 2 outside tests

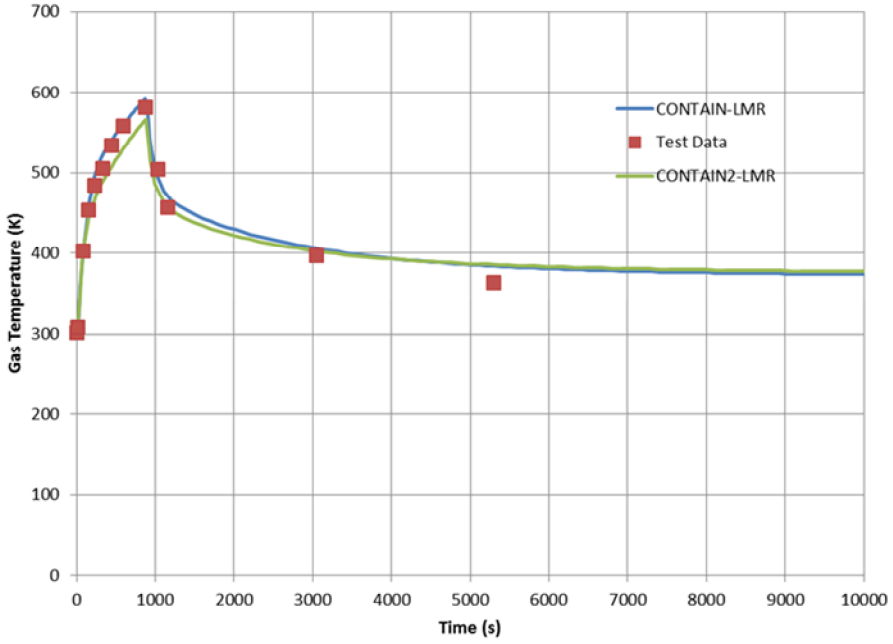
Test #	T1	T2	S1	S2
Location	In-Vessel	In-Vessel	Outside	Outside
Height of Spray (m)	5.3	5.3	4.6	4.6
Amount of Na (kg)	20	20	4	4
Flow rate (kg/s)	1	1	1	0.5
Median Particle Size Diameter (mm)	between 3 and 5	between 3 and 5	~6	~10
Initial Temperature of Sodium (deg C)	200	500	500	500
Measured Peak Air Temperature (TC's 1 foot from vessel wall for in-vessel and center of spray for outdoor tests) (deg C)	480	1200	>1200**	880
Measured Peak Vessel Overpressure (MPa)	0.006	0.2*	NA	NA
Measured Peak Narrow View Heat Flux (4.8 ft from center of vessel) (kW/m^2)	<1	89	250	40
Notes		*Instrumentation port failure	** TC failed around 1200C	

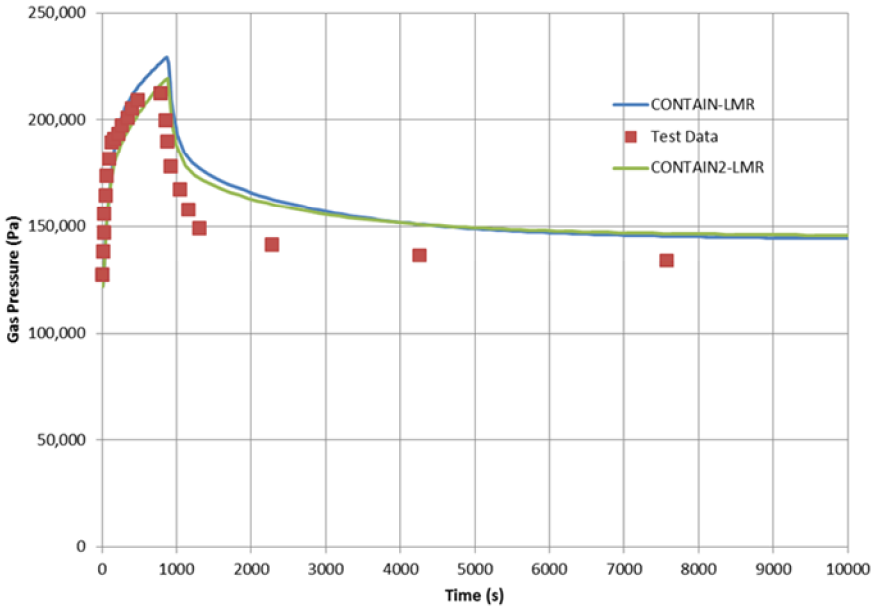
Sodium Pool Fire Models

- Sodium pool fires
  - Simulates the chemical reaction between sodium located in a pool and the oxygen in the atmosphere above the pool.
  - Based on SOFIRE II code
    - Verify against simple experiments (large test vessel)
    - CSTF AB1, AB2
  - Validate against Sandia Sodium pool fire tests (2011)
    - Varied pool depth
    - Varied pool diameter

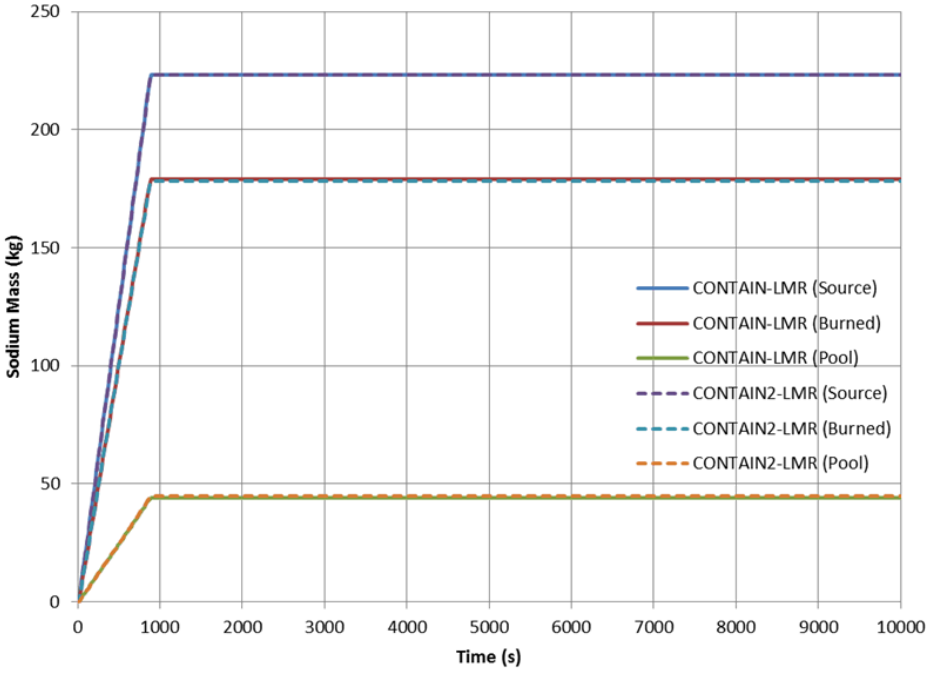
Test Number	diameter of pan (in)	height of pan (in)	mass sodium (kg)	base steel thickness (in)	average peak temperature at bottom of pan (deg C)	thickness ratio (liquid sodium/stainless steel)
pan 1	24	2	2.6	0.625	320	0.7
pan 2	24	2	2.6	0.625	320	0.7
pan 3	12	5	4.4	0.25	800	11.5
pan 4	8	7	1	0.25	780	5.9
pan 5	24	2	3.8	0.625	400	1.0
pan 6	24	2	4.8	0.625	480	1.3
pan 7	24	2	7.8	0.625	600	2.0
pan 8	24	2	1.6	0.625	220	0.4
pan 9	24	2	6	0.625	490	1.6
pan 10	24	2	11.6	0.625	746	3.0
pan 11	24	2	9.6	0.625	648	2.5

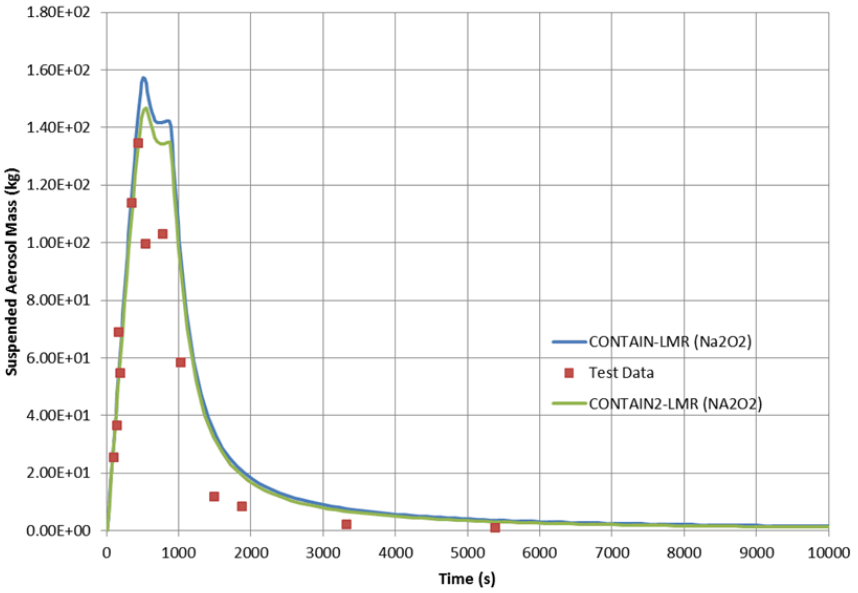
Results of Validation of AB5





Results of Validation of AB5





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