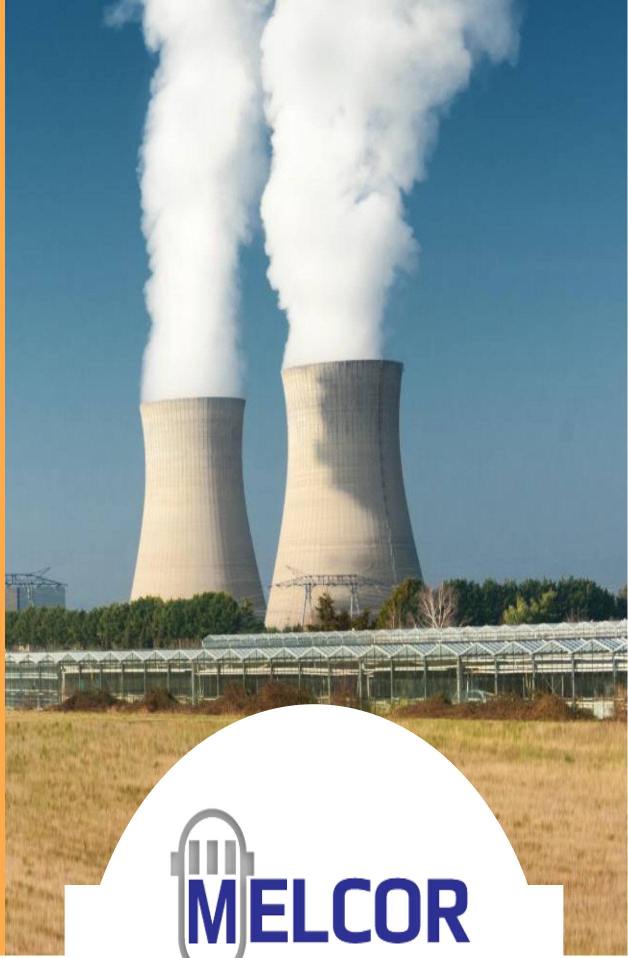
Securing the future of Nuclear Energy



Sodium Fire Validation – ABCOVE AB5/AB6/AB7

2025 European MELCOR Users' Group Meeting

April 7th-11th, 2025

SAND2025-04005PE

Overview

MELCOR NAC (sodium chemistry) package

ABCOVE

- Program description
- Series tests AB1, AB5, AB6, and AB7

Most recent MELCOR analyses and experimental validations (AB5, AB6, and AB7)

AB1 pool fire MELCOR analysis and validation

Summary

NAC Package – Sodium Chemistry

"Sodium Chemistry" – NAC – package in MELCOR

A number of reactions:

- $\mathrm{Na(l) + H_2O\ (l)\ \rightarrow NaOH(a) + \frac{1}{2}H_2}$
- $\mathrm{2Na(g,l) + H_2O\ (g,l)\ \rightarrow Na_2O(a) +\ H_2}$
- $\mathrm{2Na(g,l,a) + \frac{1}{2}O_2\ or\ O_2 \rightarrow Na_2O(a)\ or\ Na_2O_2(a)}$
- $\mathrm{Na_2O_2(a) + 2\ Na(g,l) \rightarrow 2\ Na_2O(a)}$
- $\mathrm{Na_2O(a) + H_2O\ (g,l)\ \rightarrow 2NaOH(a)}$
- $\mathrm{Na_2O_2(a) + H_2O\ (g,l) \rightarrow 2NaOH(a) + 0.5O_2}$

Kinetics of atmosphere gases not explicitly modeled

Reactions assumed to occur in hierarchal order:

- As listed above
- By reaction site (atmosphere in CV,aerosol form, surfaces such as for heat structures)

Outputs – Rxn number and energy, byproducts (Na classes, H_2), gas/liquid consumed (Na, H_2O, O_2)

NAC Package – Pool Fires

Pool fire modeling based on SOFIRE-II

- Reactions:
  - $2\,\mathrm{Na} + \mathrm{O_2} \rightarrow \mathrm{Na_2O_2}$, 10.97 MJ/kg
  - $4\,\mathrm{Na} + \mathrm{O_2} \rightarrow 2\,\mathrm{Na_2O}$, 9.05 MJ/kg
  - Half of heat produced is assigned to pool, other half is assigned to atmosphere above pool
- Reactions depend on oxygen diffusion: $D = \left(6.4315 * 10^{-5}/P\right)\left(T^{1.823}\right)$
- Input requirements:
  - F1 – fraction O_2 consumed for $\mathrm{Na_2O}$, F2 – fraction reaction heat to pool
  - F3 – fraction $\mathrm{Na_2O_2}$ to pool, F4 – fraction of $\mathrm{Na_2O}$ to pool

Quantities calculated:

- Masses consumed: Na(pool), O_2
- Masses produced: Na_2O_2+Na_2O
- Energy of reactions

Model Extensions

- Radiation between HS and pool surfaces
- Heat transfer between pool and atmosphere
  - CONTAIN/LMR uses film temperature for many thermodynamic properties.
- User-controllable pool surface area (control function)

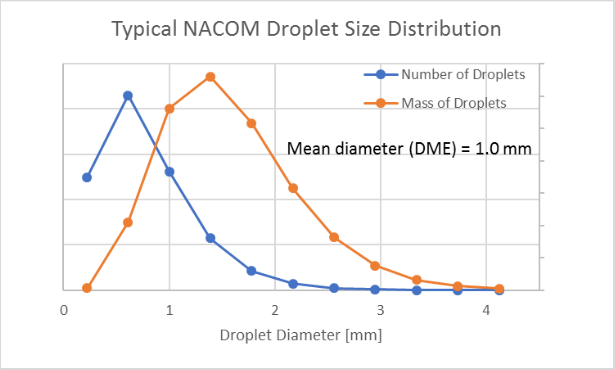
NAC Package – Spray Fires

Spray fire modeling based on NACOM (BNL)

- Inputs: fall height, mean diameter, and spray source
  - Predict whether droplet is entirely consumed over fall height
  - If consumed, add combustion and sensible energy plus energy of evaporation to atmosphere
  - If not consumed, perform time integration over droplet fall (compute diameter, velocity, temperature)
- Droplet size distribution calculated from Nukiyama-Tanasawa correlation (11 size bins)
- Droplet combustion models include pre-ignition and ignition
- Extensions to model include droplet acceleration and adjustments to heat of combustion
- Physics omitted include maximum droplet size, radiation from droplets, and swarm effects

Reactions

- (S1) $2\,Na + {}^{1}/_{2}\,O_2 \rightarrow Na_2O$,
- (S2) $2\,Na + O_2 \rightarrow Na_2O_2$



Fixed ratio of peroxide and monoxide $\left(\frac{1.3478 \cdot F_{Na_2O_2}}{1.6957 - 0.3479 \cdot F_{Na_2O_2}}\right)$

Predicted quantities include:

- Mass consumed: Na(pool), O_2
- Mass produced: Na_2O_2+Na_2O
- Energy of reactions

NAC Package – Spray Fires

Pre-ignition phase

- Na reacts with O_2 when droplet temperature cannot sustain vapor-phase burning
- Controlled by O_2 diffusion to droplet surface
- Heat-mass transfer analogy

Vapor-phase burning as droplet temperature approaches sodium boiling temperature

- Reaction heat transferred to droplet
- Balanced by heat exchange to surrounding gas by natural convection
- Leads to ignition delay for colder injection

Ignition phase

- Burning rate is based on the D2- law: $D^2 = D_I^2 - Kt$
- Burning rate of a stationary droplet: $BR_0 = \frac{\pi}{4}\rho_{Na}KD$
- Where the vapor-phase burning coefficient K is taken from Spalding: $K = \frac{8k_g}{cC_{p,g}\rho_{Na}} ln(1 + B)$
- With the transfer coefficient B: $B = \frac{1}{h_{fg}}\left(C_{p,g}\left(T_g - T_{Na}\right) + h_{com}\frac{Y_{O2}}{i}\right)$
- Adjustment made for forced convection: $BR = BR_0\left(1 + C_f Re^{1/2} Pr^{1/3}\right)$

NAC Package – Spray Fires

Droplet velocity models

- Terminal velocity – downward sprays only
  - Droplet fall time approximated from user specified fall height and terminal velocity
  - Assume droplet Immediately accelerates to terminal velocity
- Acceleration – upward or downward sprays
  - User can specify upward spray with a negative initial velocity (positive assumed downward)
  - Velocity

$$\frac{\mathrm{dv}}{\mathrm{dt}} = \mathrm{g} - \mathrm{drag(v)}$$

  - Drag

$$\mathrm{drag(v)} = \frac{3}{4} * \frac{\rho_g}{\rho_l * d} * \mathrm{v} * \mathrm{abs(v)} * C_d(\mathrm{Re})$$

  - Height

$$h(\mathrm{t}) = h(t - \Delta t) - \mathrm{v}(t - \Delta t) * \Delta t$$

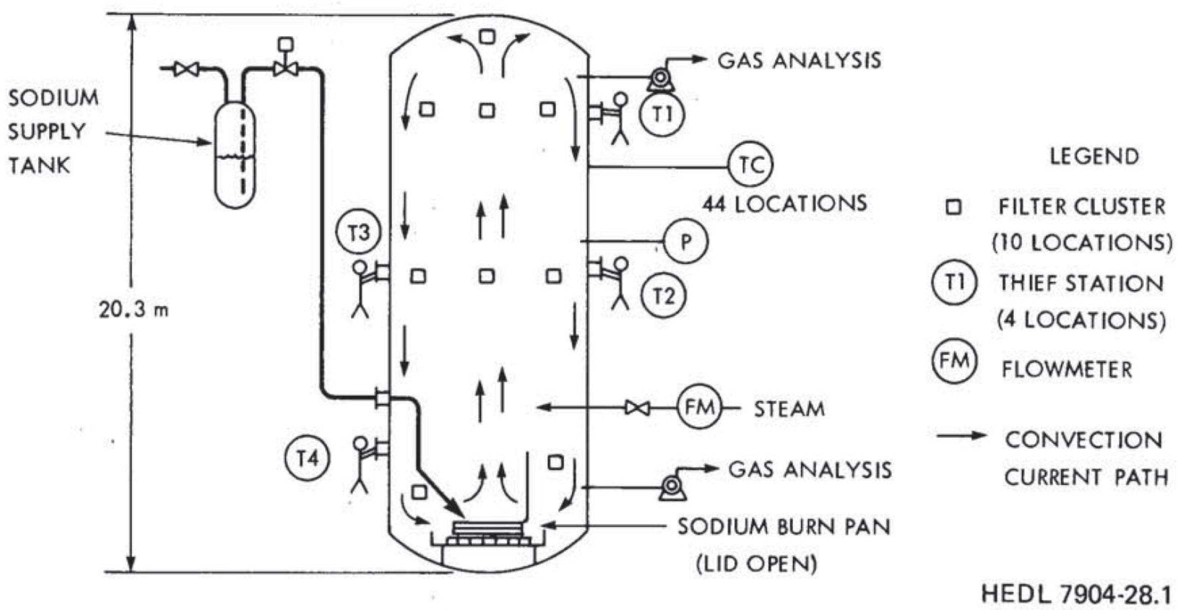
ABCOVE Program

Purpose:

- Judge adequacy of aerosol transport codes in describing aerosol behavior in containment
- Utilize Containment Systems Test Facility (CSTF) at Hanford Engineering Development Laboratory
- Establish technical basis for analyzing accidents involving sodium spray and pool fires

Large-scale experiments in containment vessel of CSTF, including:

- AB1 – 1979 – “Dry” aerosols (NaOH, Na_2CO_3, Na_2O_2) generated from pool fire, aged in containment
- AB5 – 1982 – Single-species aerosol generated by high-rate sodium spray into air atmosphere
- AB6 – 1983 – NaI aerosol released in presence of a sodium spray fire
- AB7 – 1984 – NaI aerosol released upon conclusion of a small sodium pool fire



ABCOVE AB5

Moderate duration, strong aerosol source

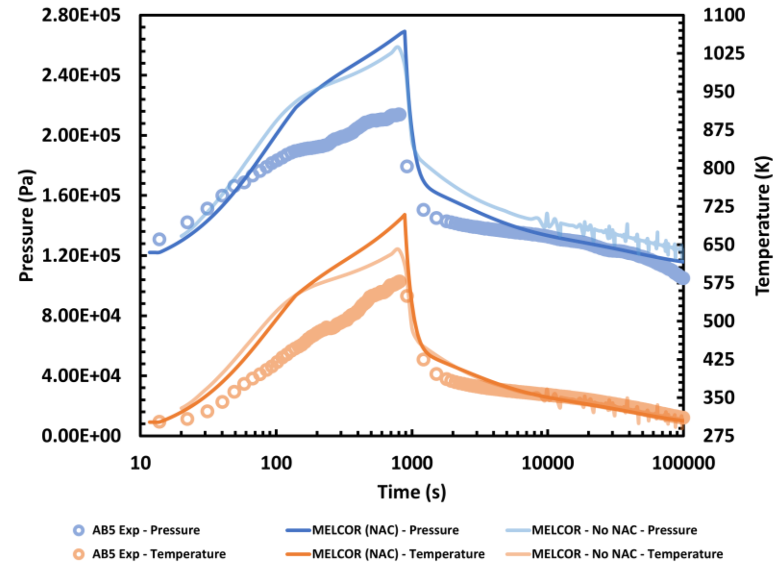
Spray fire in air atmosphere - 13 s to 885 s

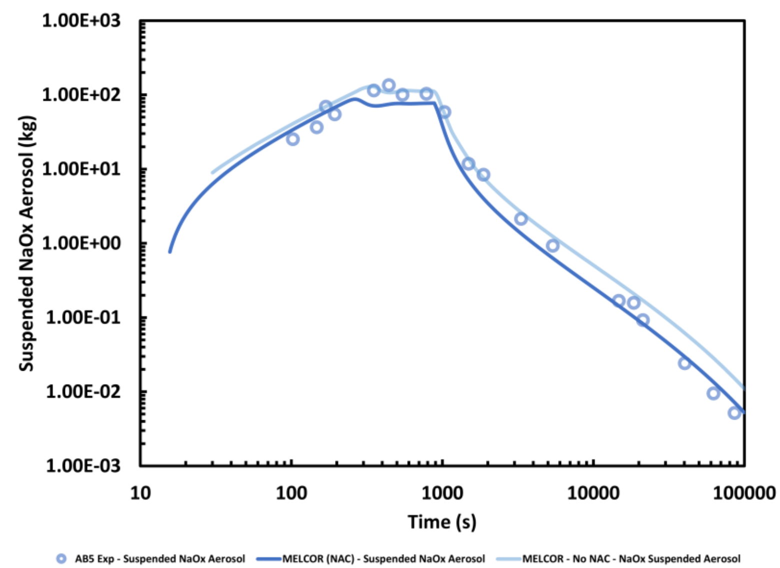
- Aerosols created: NaOH, Na_2O, Na_2O_2
- H_2O in air atmosphere drives NaOH generation
- 223 kg integral Na mass

MELCOR predictions

STRUCTURE	...	MELCOR	...	MELCOR-NAC					...	TEST AB5
Plated Mass	...	**NaOx (kg)**	...	**NaOH (kg)**	**+**	**Na2O2 (kg)**	**=**	**NaOx (kg)**	...	**NaOx (kg)**
Top Head	...	1.60	...	0.50	+	1.63	=	2.13	...	0.96
Cylindrical Walls	...	18.10	...	1.41	+	5.51	=	6.92	...	17.75
Internal Components (Vertical)	...	3.82	...	2.15	+	4.97	=	7.12	...	N/A
Total Plated*	...	23.52	...	4.06	+	12.11	=	16.17	...	18.70
Settled Mass	...	**NaOx (kg)**	...	**NaOH (kg)**	**+**	**Na2O2 (kg)**	**=**	**NaOx (kg)**	...	**NaOx (kg)**
Bottom Head	...	190.00	...	22.82	+	141.14	=	163.96	...	200.10
Internal Components (Horizontal)	...	176.50	...	21.42	+	132.51	=	153.93	...	184.00
Total Settled^	...	366.50	...	44.24	+	273.65	=	317.89	...	384.10
Total Deposited	...	390.02	...	48.30	+	285.76	=	334.05	...	402.80

- Over-predicting containment atmosphere P/T
  - Combustion flame radiation to HS surfaces?
  - Vigorous aerosol generation might lessen the effect
  - Could result in more energy to atmosphere vs. HS
- Good prediction of aerosol mass generation





ABCOVE AB6

Coagglomeration of two aerosol species

Spray fire in air atmosphere - 620 s to 5400 s

NaI aerosol injected 0 s to 3000 s

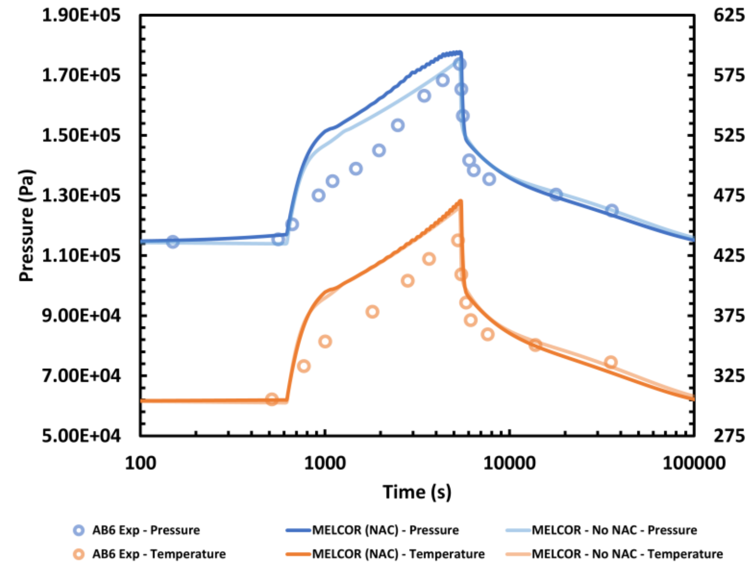
- Aerosols created: NaOH, NaI, Na_2O, Na_2O_2
- H_2O in air atmosphere drives NaOH generation
- 204.7 kg integral Na mass, 420 g integral NaI mass

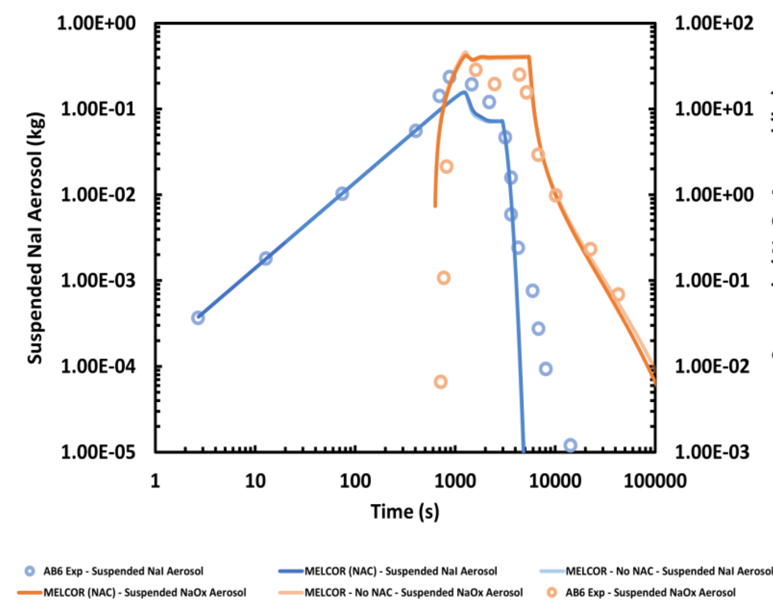
MELCOR predictions

STRUCTURE	...	MELCOR		...	MELCOR-NAC						...	TEST AB6	
Plated Mass	...	**NaOx (kg)**	**NaI (g)**	...	**NaOH (kg)**	**+**	**Na2O2 (kg)**	**=**	**NaOx (kg)**	**NaI (g)**	...	**NaOx (kg)**	**NaI (g)**
Top Head	...	0.40	0.38	...	0.05	+	0.40	=	0.46	0.38	...	1.58	1.68
Cylindrical Walls	...	11.00	13.00	...	1.51	+	11.23	=	12.75	14.62	...	35.80	46.51
Internal Components (Vertical)	...	1.28	2.85	...	0.50	+	1.25	=	1.75	3.82	...	N/A	N/A
Total Plated*	...	12.68	16.23	...	2.07	+	12.89	=	14.96	18.82	...	37.38	48.19
Settled Mass	...	**NaOx (kg)**	**NaI (g)**	...	**NaOH (kg)**	**+**	**Na2O2 (kg)**	**=**	**NaOx (kg)**	**NaI (g)**	...	**NaOx (kg)**	**NaI (g)**
Bottom Head	...	186.00	209.00	...	14.49	+	145.07	=	159.56	203.91	...	156.07	195.60
Internal Components (Horizontal)	...	172.00	195.00	...	13.70	+	148.50	=	162.21	192.96	...	179.00	172.60
Total Settled^	...	358.00	404.00	...	28.20	+	293.57	=	321.77	396.87	...	335.07	368.20
Total Deposited	...	370.68	420.23	...	30.27	+	306.46	=	336.73	415.69	...	372.45	416.39

* --> 30% error, ^ --> 10% error

- More mild fire (less flame-to-HS effect?)
- Greater sensitivity to gas injection alongside NaI
- Good prediction of aerosol mass generation





ABCOVE AB7

Coagglomeration of two aerosol species under mild thermal conditions (min resuspension, decomposition)

Na leak out of tube - 0 s to 20 s

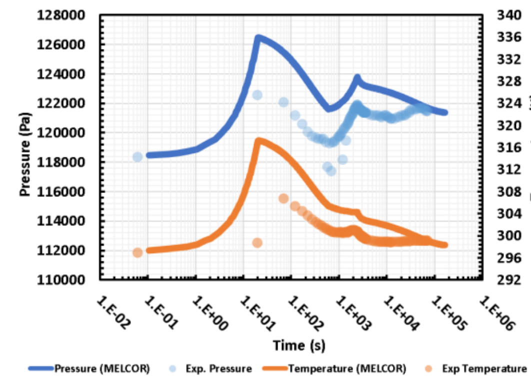
Na accumulation on platform, pool fire 20 s to 600 s

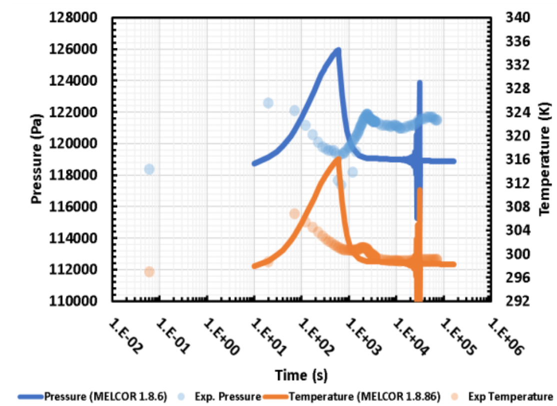
NaI aerosol injected 600 s to 2400 s

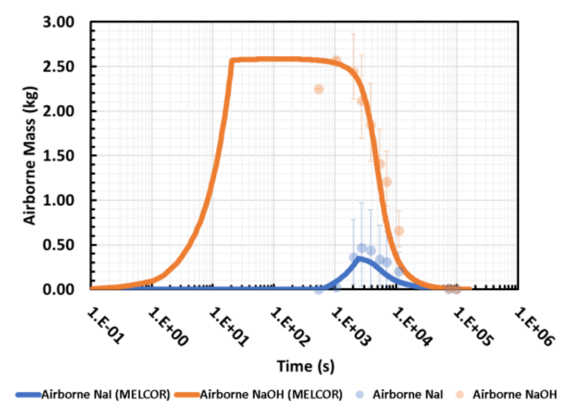
- NaOH produced immediately after leak
- H_2O in air atmosphere drives NaOH generation
- 6.434 kg integral Na mass, 354.6 g integral NaI mass

MELCOR predictions

- Able to capture relatively “small” event
- Much uncertainty about experimental conditions
  - Leak resembled a flow more than a spray
  - Flow dripped to I-beam then dripped to platform
- MELCOR 2.X analysis improved over MELCOR 1.8.6
- Good prediction of airborne mass







ABCOVE AB1

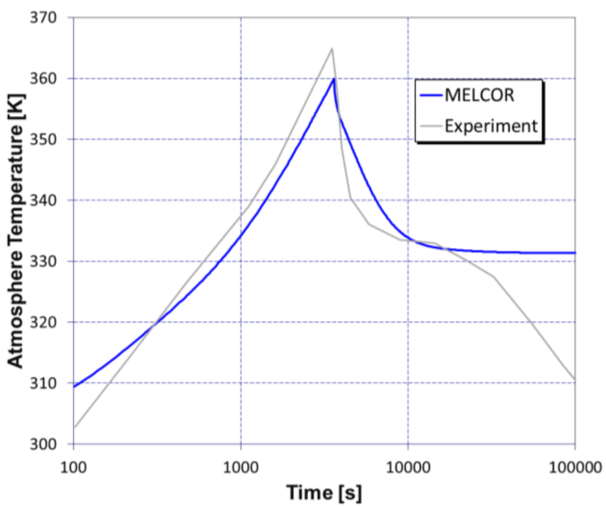
Characterize aerosols from pool fires (dry atmos)

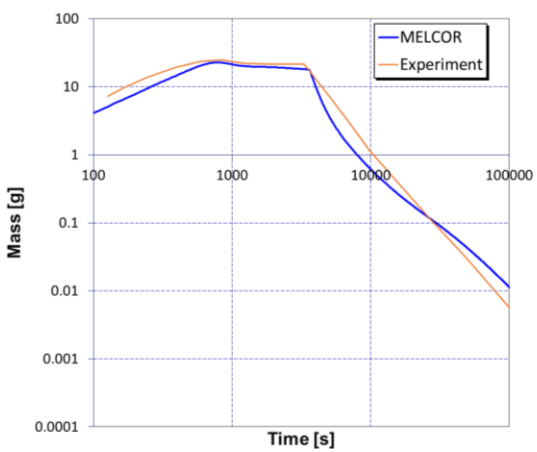
Evaluate P/T response of containment atmosphere

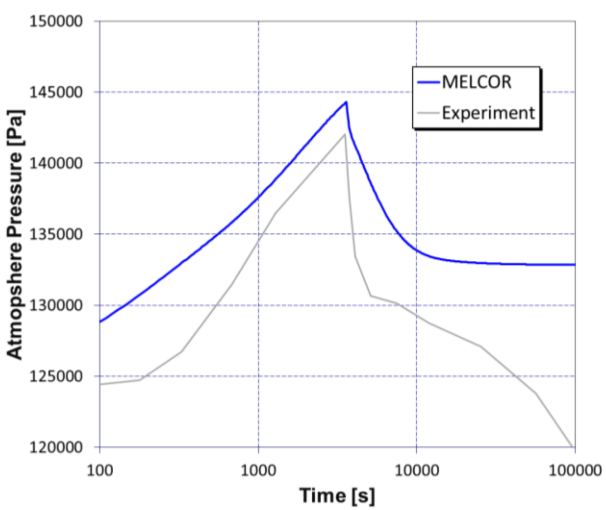
Spill 410 kg Na at 600 C in a 4.4 m^2 pan, burn 3600 s

MELCOR Predictions

- Fair agreement on P/T atmosphere response
- Good prediction of airborne aerosol mass through the aerosol release period and thereafter







Summary

Reviewed NAC package models/capabilities

- Sodium chemistry
- Pool fire models
- Spray fire and droplet models

Reviewed most recent validation/benchmark calculations – ABCOVE AB5/6/7

Reviewed ABCOVE AB1 pool fire analysis