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Benchmarking MELCOR's NAC Package to ABCOVE Test AB7

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ABSTRACT

This report presents analyses of the AB7 ABCOVE sodium spray fire experiment with the MELCOR code. This code simulates the progression of accident events for analysis and auditing purposes of nuclear facilities during accident conditions. Historically, the ABCOVE experiments have contributed to the validation of aerosol physics and related phenomena. Given advancements in sodium-cooled reactor designs, characterization of the sodium spray combustion may further the review and validation of newly incorporated sodium properties and physics packages, namely, the sodium equations of state (EOS) and the sodium combustion (NAC) package within MELCOR. Previously, the AB5 and AB6 experiments were analyzed with and without the NAC package. This work builds on the previous analyses with a demonstration of the current code capabilities of MELCOR with a more mild Na spray and pool fire scenario.

Acknowledgment

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Nomenclature

ABCOVE Aerosol Behavior COde Validation and Evaluation

AMMD Aerosol Mass Median Diameter

CSTF Containment System Test Facility

CV Control Volume

CVH Control Volume Hydrodynamic

CVT Control Volume Thermodynamic

DCH DeCay Heat

DOE Department of Energy

EOS Equations Of State

GSD Geometric Standard Deviation

JAEA Japan Atomic Energy Agency

LACE Light water reactor Aerosol Containment Experiment

LMFBR Liquid Metal Fast Breeder Reactor

LMR Liquid Metal Reactor

LWR Liquid Water Reactor

MMDD Mass Median Droplet Diameter

MELCOR MELting CORe

NAC Na Chemistry

NCG Non-Condensible Gas

NRC Nuclear Regulatory Commission

RN Radio-Nuclide

SFR Sodium Fast Reactor

SNAP Symbolic Nuclear Analysis Package

SNL Sandia National Laboratories

1. ABCOVE OVERVIEW

Severe accident scenarios at a nuclear power plant often result in the subsequent release of substantial amounts of radioactive aerosolized particulate. These particles can contain materials from a melted core or could be a part of flammable components such as molten sodium. Aside from noble gases and select iodine compounds, the behavior of these radioactive aerosol compounds requires more characterization. Being able to better understand and predict the behavior of these particulates in the event of a severe accident is vital to understanding the consequences of a possible release of material. To predict many of the chemical and physical phenomena that affect and/or contribute to aerosol behavior under severe accident conditions, computer codes were developed and compared against experimental data sets [1, 2].

In 1994, Francisco Souto performed an assessment covering tests from the aerosol behavior code validation and evaluation (ABCOVE) program and light water reactor aerosol containment experiments (LACE) using MELting CORe (MELCOR) 1.8.2 [3]. His assessment encompassed four separate experiments: AB5, AB6, AB7 and LA2. The ABCOVE program, which utilized the containment systems test facility (CSTF) located at the Hanford Engineering Development Laboratory (HEDL), served to provide a technical basis for the applicability of various aerosol behavior codes for accidents within containment buildings involving molten sodium. This program attempted to compare the results acquired from large-scale experiments in the CSTF with the analytical calculations performed by code developers to view the fidelity and/or discrepancies within each tested code set. Similarly, the LACE program investigated aerosol retention behavior for theorized, high-consequence accident scenarios in order to provide a dataset for validating aerosol and thermal-hydraulic computer codes revolving around light water reactors [1, 2, 3, 4]. Since the interests of this work are toward the behavioral data of aerosol in liquid-metal cooled reactors or more particularly, sodium fast reactors (SFRs), the reader is guided to [3] for further discussion on the LACE program.

Since the ABCOVE program, there has been a drive to close the gap on sodium spray fire knowledge as advanced nuclear reactors are entering their developmental/prototyping phase within the next few years. Some of these advanced reactors aim to use liquid sodium as their source of coolant however, knowledge about the effects of Na combustion in aerosol species transport from a molten sodium a leak/spray accident is not well understood. Thus, series of experiments have been performed both locally at Sandia National Laboratories (SNL) and at the Japan Atomic Energy Agency (JAEA) [5, 6] to try to validate data streams between experimental datasets and computational predictions. Some early successes were recorded in both experiments [5, 6] using codes such as CONTAIN-LMR [7] and SPHINCS [8]. Over time, these codes have been modified and changed. Sodium models available in CONTAIN-LMR were incrementally adapted to fit into the MELCOR code into what it is now today, the NAC

package [9, 10]. Like MELCOR, these codes operate on the use of control volumes to move heat, masses and aerosols about the modeled system (see Figure 1-1).

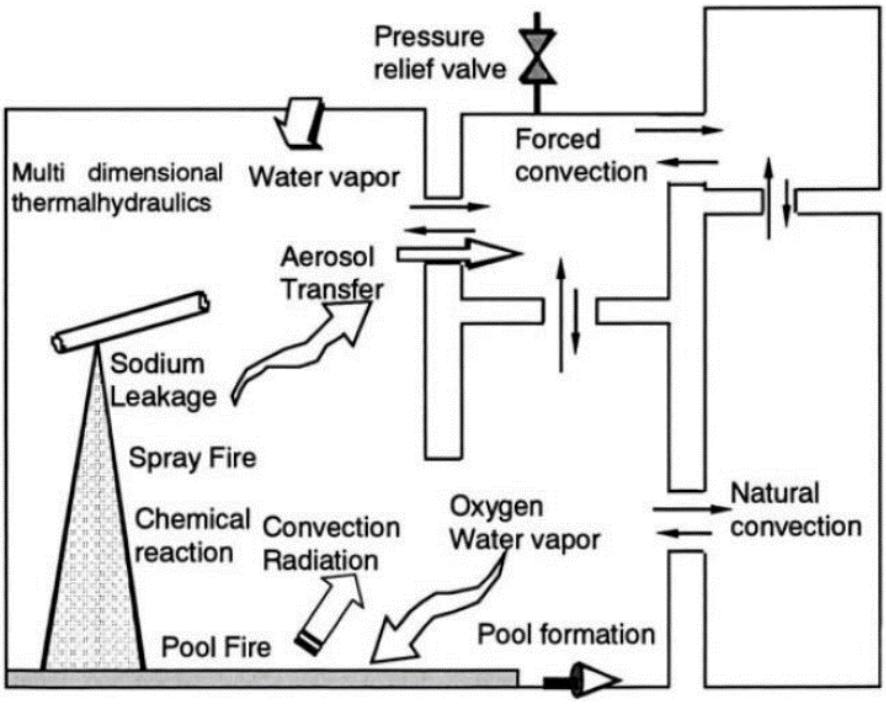

Figure 1-1. Models used in the SPHINCS and CONTAIN-LMR computer codes [11]. The partitions represent the separation of cells that can be used to model the transport of fluids between cells.

Historically, the AB5/AB6 experiments have contributed to the aerosol code validation for MELCOR however, analyses of the code results have yet to be performed using the sodium combustion (NAC) package and/or the sodium equation of state (EOS). Given the advancement of the MELCOR code to incorporate direct modeling of combustion phenomena, code users may use either the traditional modeling approach or the NAC package, when deemed appropriate. Prior to the NAC package, code users, such as Souto [3], modeled the effects of sodium combustion events through direct sourcing of the source term. This involves the use of tabular functions throughout the MELCOR input deck that represent Na insertion and subsequent aerosol formation over time via: the input Na mass flow rate, the temperature of that Na mass, and the aerosol formation over time. Note, modeling the source term in this fashion requires extensive source term characterization that incorporates: release initiation, elevation and duration, thermal-dynamic and thermal hydraulic conditions to assist in plume characterization, and additionally, the size distribution and composition of the released materials. Given a postulated release of sodium from a SFR coolant system, the reaction between the sodium and available oxygen and/or water vapor results in the formation of sodium oxides, hydroxides and peroxides where each of these reactions subsequently generate a substantial amount of heat. The estimated amount of heat must also be imported into the model as a heat source. These exothermic reactions can drive pressure and temperature increases in containment vessels, leading to a possible failure event. Thus, characterizing source terms, material released from a containment and/or confinement to the outside environment, requires modeling the effects of the thermal and

pressure loading upon the facility as well as the transportation and interaction of the aerosols formed via sodium combustion products with other available aerosols like water vapor/oxygen and any released fission products.

Rather than importing experimental data regarding the behavior and formation of combustion aerosols, the NAC package attempts to wholly model the combustion behavior of Na through three scenarios: spray and pool fire incidents and atmospheric chemistry. The NAC package is targeting predictive behavior capabilities to assist in the safety analysis for the development of sodium-cooled fast reactors. This report will review the aerosol experiment, AB7, and perform an analysis on the modeled sodium spray and pool fire behavior using MELCOR's NAC package. Test AB7 utilized the CSTF containment vessel whose dimensions, weight, surface areas and material thicknesses can be found in Table 1-1. Some comparison and discussion will be made against the traditional method used in MELCOR. Future endeavors will include comparisons with a JAEA developed code, SPECTRA, analyzing the same tests.

Table 1-1. CSTF Containment Vessel Properties [3].

DIMENSIONS	
Diameter (ID)	7.62m
Total Height	20.3m
Cylinder Height	16.5m
Enclosed Volume	852m^3
WEIGHT	
Top Head	8753kg
Bottom Head	8753kg
Cylinder	69390kg
Penetrations and Doubler Plates	10295kg
Catch Pan	500kg
Internal Components	5580kg
Total Weight	103260kg
SURFACE AREAS FOR HEAT TRANSFER	
Top Head	63.0m^2
Bottom Head	63.0m^2
Cylinder	394m^2
Total CSTF Vessel Shell	520m^2
Internal Components	232m^2
SURFACE AREAS FOR AEROSOL SETTLING	
Bottom Head	36.7m^2
Catch Pan	11.1m^2
Personnel Deck	4.2m^2
Internal Components	36.2m^2
Total	88.2m^2
SURFACE AREAS FOR AEROSOL PLATING	
Vessel Shell	520m^2
Internal Components	232m^2
Total	752m^2
THICKNESS FOR HEAT TRANSFER (AVERAGE LUMPED)	
Top Head	18.1mm
Bottom Head	18.1mm
Cylinder	22.9mm
Internal Components	3.4mm

1.1. AB7

Test AB7 was performed in September 1984 at HEDL. This test involved the release of a fission product simulant, NaI, after the end of a small pool fire caused by a Na pipe leak [12]. The purpose of this test was to demonstrate the coagglomeration behavior of two aerosol species under mild thermal conditions. The released Na was small enough that re-suspension and decomposition processes were negligible. The test setup for AB7 of the ABCOVE program is shown below.

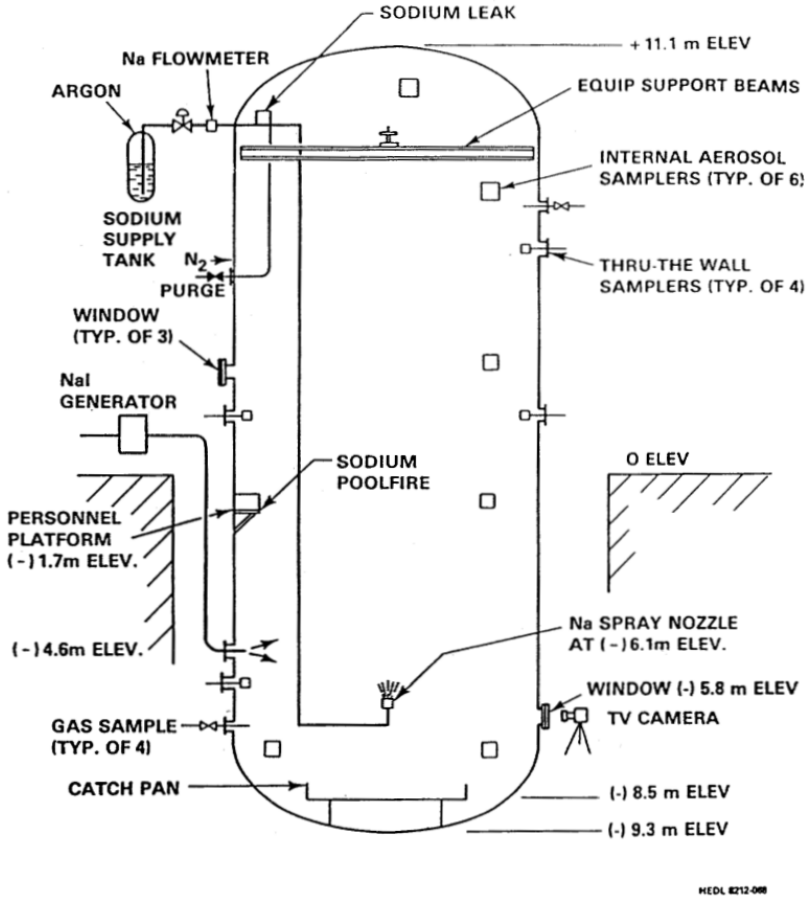

Figure 1-2. Setup of the CSTF containment vessel for AB5 [3].

For this test, 6.434 kg of commercial-grade, molten sodium leaked out from an 11mm diameter pipe at the top of the CSTF containment vessel, made contact with the equipment support beams, and fell onto a personnel platform for a period of 20s. During the leak period, aerosol formation through Na combustion was observed and quantified. A pool fire was also noted to have accumulated and burned from 20s to 600s on the personnel platform. From 600s to 2400s, NaI was injected into the system with a N_2 carrier gas. Analysis from the end of the experiment concluded the conversion of sodium through combustion resulted in the generation of nearly 100% NaOH aerosol due to the low amount of Na released and moisture in the atmosphere. Note, the containment vessel was kept sealed for 44 hours from time t=0s. Then an air purge was

performed where at 45 hrs past t=0s, the CSTF was entered and samples were taken. A summary of the experimental conditions can be found in Table 1-2.

Table 1-2. Summary of Test AB7 conditions [3].

TEST CONDITION	VALUE
Initial Containment Atmosphere	
Oxygen Concentration	20.95%
Temperature (mean)	297.05K
Pressure	118.4kPa
Dew Point	274.65K
Sodium Spill	
Sodium Flow Rate	322g/s
Sodium Flow Duration	20s
Sodium Fall Distance	10m
Sodium Mass Delivered	6.434kg
Initial Sodium Temperature	863.15K
Pool Fire Burning Area	$0.93m^2$
Pool Fire Burn Duration	600s
Containment Conditions During Test	
Maximum Average Atmosphere Temperature	306.85K
Maximum Average Steel Vessel Temperature	298.35K
Maximum Pressure	122.6kPa
Final Dew Point	274.45K
NaOH Aerosol Source	
Start Time	0s
Stop Time	600s
Release Rate	5.03g/s
Total NaOH Released	3.018kg
Material Density	$2.13g/cm^3$
Source 50% Diameter	0.5µm
Source Geometric Standard Deviation	2.0
Mass Ratio, NaOH to Na	1.74
NaI Aerosol Source	
Start Time	600s
Stop Time	2400s
Release Rate	0.197g/s
Total NaI Released	354.6g
Material Density	$3.67g/cm^3$
Source 50% Diameter	0.54µm
Source Geometric Standard Deviation	1.55

The temperature/pressure and aerosol data serve to provide validation data for computational codes that model containment response and aerosol behavior, respectively. The aerosol experimental data can be categorized into five relevant output types for code validation: airborne mass, settled mass, plated mass, aerodynamic mass median diameter, and the geometric standard deviation of the particle size distribution. The validation of thermal-hydraulic code for this test relies on the pressure and temperature experimental data obtained from containment and atmospheric measurements.

2. MELCOR

MELCOR is a fully integrated, engineering-level computer code that provides the capability to model the progression of severe accidents in light water reactors within nuclear power plants. This code has been supporting the United States Nuclear Regulatory Commission (NRC) since its original design as a second-generation plant risk assessment tool in performance of source terms estimations for severe accidents and encompassing sensitivities as well as uncertainties across a multitude of applications. MELCOR was originally designed to analyze severe accidents that may occur within LWR technologies such as thermal-hydraulic response in the reactor coolant system, reactor cavity, containment, and confinement buildings; core heat-up, degradation, and relocation; core-concrete attack; hydrogen production, transport, and combustion; fission product release and transport behavior [13]. Despite the original intent of the code, the capabilities have been expanding over the past decade. MELCOR is under constant development for applications following the trends in nuclear power technologies, most notably advanced reactors.

2.1. Sodium Combustion Package

To support the accident phenomena associated with sodium reactor designs, the sodium combustion (NAC) package was introduced into MELCOR. The NAC package supports sodium chemistry models associated with liquid sodium incidents, such as coolant loss events leading to spray and/or pool fires. As sodium undergoes exothermic reactions with oxygen and water in the air, the resulting energy release and the formation of sodium oxide aerosols are computed. These phenomena are crucial to perform Level 2 and 3 probabilistic analyses as well as to accurately characterize the timing and scale of any environmental release in modeled accidents in advanced sodium-cooled reactor designs.

Given the inclusion of the NAC package and sodium equation of state (EOS), the sodium modeling options have been extended to provide direct modeling capabilities for sodium application within MELCOR. Prior to these inclusions, MELCOR analyses had been previously limited to experiments with small quantities of sodium and sodium byproducts assuming the total masses could be considered negligible for the hydrodynamic solutions, i.e., the sodium related masses are sufficiently small that other materials such as noncondensible gases dominated advection computations. Therefore, prior validation analyses for sodium spray fires are suitable candidates for analyses with the extended sodium capabilities. This report discusses the sodium spray/pool fire modeling within MELCOR with an emphasis on modern methodologies for the AB7 test.

The sodium chemistry models integrated into MELCOR are based on the CONTAIN-LMR code [7], which has been developed and refined by the JAEA. The NAC package computes the

combustion rate of sodium in both spray and pool configurations, along with the interactions between water vapor, sodium vapor, and aerosols in the atmosphere. The calculated mass and energy exchange rates for sodium serve as references for the corresponding code packages. The NAC package features specific database elements that must be defined to facilitate the interfaces between the NAC and other code packages. Notably, the spray and pool geometries rely on the primary hydrodynamic materials in the control volume hydrodynamics package. The physical properties and EOS of the main hydrodynamics material are accessible to all packages upon request from the control volume thermodynamics (CVT) package.

For sodium-related analyses, users are required to designate sodium as the primary hydrodynamics material. Sodium replaces water in both the CVH and CVT packages, accomplished by selecting one of the independently developed sodium EOS data files distributed in conjunction with the MELCOR executables. For further details on the application of sodium EOS, please refer to the NAC User's Guide. The reader is also encouraged to review [14] for more detailed information on NAC input fields.

Table 2-1. Atmospheric Chemistry Reactions Data and Applications [13].

#	Reaction	Reaction Heat	Locations
1	$Na + H_2O\ (l) \rightarrow NaOH + \frac{1}{2}H_2$	$\Delta H_{NaOH} - \Delta H_{H2O}$	Reactions within aerosol particles or within aerosol deposit or condensable film
2	$2\ Na + H_2O\ (g) \rightarrow Na_2O + H_2$	$\Delta H_{Na2O} - \Delta H_{H2O}$	Reactions with gases, aerosols with gases, and deposits or film with gases
3	$2\ Na + (1 - 0.5 \cdot f_{ox})O_2 \rightarrow f_{ox} \cdot Na_2O + (1 - 0.5 \cdot f_{ox}) \cdot Na_2O_2$	$f_{ox} \cdot \Delta H_{Na2O} + (1 - f_{ox}) \cdot \Delta H_{Na2O2}$	Reactions of gases with gases, aerosols, and deposits/film
4	$Na_2O_2 + 2\ Na \rightarrow 2\ Na_2O$	$\Delta H_{Na2O} - 0.5\ \Delta H_{Na2O2}$	Contact reactions within an aerosol particle or within aerosol deposits or condensable film. aerosol reaction with excess sodium in the atmosphere, and aerosol reactions on the film
5	$Na_2O + H_2O\ (g) \rightarrow 2\ NaOH$	$\Delta H_{NaOH} - 0.5\ (\Delta H_{Na2O} + \Delta H_{H2O})$.	Reactions within a repository, such as within an aerosol, aerosol deposit or condensable film, reactions of aerosol with gas, and reacting deposits or film with gases
6	$Na_2O_2 + H_2O\ (g) \rightarrow 2\ NaOH + \frac{1}{2}O_2$	$\Delta H_{NaOH} - 0.5(\Delta H_{Na2O2} + \Delta H_{H2O})$	

As the NAC package currently exists, only reactions 3 and 6 in Table 2-1 are functional in the code. This creates a limitation on the actual behavior of the aerosol speciation. Ideally, having competing reactions in the system would better model reality and provide more accurate predictions.

3. RESULTS & DISCUSSION

A previous AB7 model [3] created using MELCOR 1.8.2 was converted to MELCOR 1.8.6 using SNAP [15], and executed using MELCOR 1.8.6. This was done to maintain the same code comparison as in the original analysis [3]. The NAC-enabled model was built and executed using MELCOR 2.2 (r2024.0.0) to provide a direct code-to-code comparison of the traditional MELCOR methodology of sourcing in all Na aerosol species and energy into the system vs. today's implementation using the NAC package to determine the generation of these species in situ. When comparing several plots and tables from Souto's [3] are presented and refreshed with the added data generated from the updated MELCOR simulations using the NAC package. It should be noted that Souto's analysis involved modeling the heat structures as stainless-steel instead of carbon-steel. The updated material definition for the heat structures was implemented in the newer model. In addition, experimental results show that the overall production of Na_2O/Na_2O_2 were negligible and/or had all been converted to NaOH, therefore, it was not modeled or accounted for and was assumed to be zero for test AB7. A small difference in the modeling of the CSTF for test AB7 vs. AB5/AB6 [14] involved splitting the control volume modeling the CSTF atmosphere in two at the point where the Na spill collects and forms a pool at the personnel platform elevation. This required the splitting of the CSTF walls heat structure into an upper and lower portion.

3.1. AB7

The NAC package was used to evaluate the aerosol and energy generation characteristics of test AB7 of the ABCOVE test series. The results of this work were compared to a previous MELCOR assessment and experimental results. Plating and deposition values are outlined in Table 3-1. It was determined that Souto's analysis did not account for the Na spill effects for combustion and only considered a pool formation with a subsequent pool fire. This underestimated the pressure/temperature effects of combustion events occurring within the first 20 seconds. Souto did not consider the added heated nitrogen gas stream that acted as a carrier to the NaI aerosol which, given the minor effects in test AB7, is really noticeable in pressure and temperature responses. The pool area was also not considered and thought to have affected Souto's results providing an overestimation in the energy provided by the pool fire. The energy generation and dissipation from the use of the NAC package revealed a potential issue MELCOR's handling of combustion energy transfer with respect to flame to heat structure energy deposition. Radiative heat transfer from the combustion flame to the walls is not modeled in MELCOR and is theorized to be the primary reason for the thermal-hydraulic responses' slight overestimation as sources dictate approximately 35% of the generated heat of a fire goes directly to the surrounding heat

structures [16]. The deposition and suspension behavior of the aerosol species was agreeable when compared with experimental data.

3.1.1. Aerosol Behavior

3.1.1.1. Production Mechanisms for the NaOH Aerosol

The production mechanisms of Na-based aerosols can be found in Table 2-1. For the chemical reactions involving the *direct* production of NaOH from Na, we have the following:

$$2Na + 2H_2O \longrightarrow 2NaOH + H_2 \tag{3.1}$$

For test AB7, they determined that all the combusted Na immediately reacted with moisture in the air to form NaOH. No further data was provided for the production of other aerosol species [12]. Therefore, the production of species other than NaOH was limited in this analysis. To provide an upper boundary on the maximum amount of NaOH that could be generated, we can assume all 6.434 kg injected Na solely underwent reaction 3.1. Thus, the maximum NaOH that could be produced is 9.36 kg. In this calculation, the moisture in the atmosphere was found to be the limiting reagent with a total estimated 234 moles H_2O vapor. Experimental results, shown in Table 3-1, report 2.92 ± 0.27 kg NaOH deposited. This indicates that not all of the Na that leaked combusted and underwent a chemical reaction. This is further confirmed with the experimental identification of a pool formation. Note, the collection of Na in a pool allowed a bulk amount of Na to remain as Na metal since pool fire combustion is only occurring at the surface.

3.1.1.2. Production Mechanism for NaI Aerosol

NaI was sourced as an aerosol using the same RN1_AS and RN1_AS01 records as done in [14].

```
RN1_AS  'AS002' 'CSTF' VAPOR 'NAI'  0.0 1.97E-4   TF 'ASOURCE2'
RN1_AS01      LOGNORMAL       5.44E-7          1.55
```

To provide a more accurate analysis for NaI aerosol, a new class was added (class 22) to the RN1_CC and DCH_CL fields. This presents a difference to Souto's work where CsI was used as a surrogate for NaI, however, the mass of Cs is 5.78 times heavier and was thought to affect the aerosol behavior for this work. Thus, a new class was added to accommodate the inherent vapor pressure and molecular weight differences of NaI compared to CsI. In addition, a heated N_2 carrier gas was defined as a control volume source with a simultaneously release time as the NaI source. Unlike the previous analysis [14] which utilized exact data from [1], this work had to make a proportional approximation to the amount of N_2 gas inserted in the system since [12] does not report it. The proportion was taken for AB7 data against the amount and rate of NaI with N_2 gas inserted in test AB6.

3.1.1.3. Deposition of Aerosols onto Heat Structures

The results of the deposited aerosol species onto the heat structures ('top-head', 'cylindrical walls', 'internal components (vertical)', 'bottom-head' and 'internal components (horizontal)') are shown in Table 3-1 below. The results of the plated and settled aerosol species of NaI and NaOH were mostly consistent with the previous MELCOR results with some caveats: the plated and settled masses for the NAC-enabled MELCOR simulations were under-predicted compared to the experimental dataset while the plated and settled masses for the MELCOR 1.8.6 simulations were slightly over/under predicted, respectively.

Table 3-1. ABCOVE test AB7 deposition results comparison between MELCOR 1.8.6 [9], MELCOR 2.2 with NAC-enabled, and test AB7 experimental data.

STRUCTURE	**MELCOR 1.8.6**		**MELCOR-NAC**		**TEST AB7**	
Plated Mass	**NaOH (g)**	**NaI (g)**	**NaOH (g)**	**NaI (g)**	**NaOH (g)**	**NaI (g)**
Top Head	0.22	0.0039	1.34	0.00178	18	1
Cylindrical Walls	19	2.5	123	2.83	130	4.1
Internal Components (Vertical)	9	1.25	45.6	1.40	87	3.85
Total Plated*	28.2	3.75	170.61	4.23	235	8.95
Settled Mass	**NaOH (kg)**	**NaI (kg)**	**NaOH (kg)**	**NaI (kg)**	**NaOH (kg)**	**NaI (kg)**
Bottom Head	1.54	0.18	1.26	0.133	1.24	0.18
Internal Components (Horizontal)	1.44	0.17	1.18	0.201	1.44	0.234
Total Settled^	2.98	0.35	2.434	0.334	2.68	0.414
Total Deposited	3.01	0.354	2.604	0.338	2.92	0.423

Experimental Error: *30 %, ^10%

There were several noted differences such as those found in the settled masses. Because the NAC-enabled MELCOR simulation utilizes Na as its working fluid and actually propagates Na reactions, there is a chance for a percentage for the Na to not combust. Droplet combustion was incomplete for certain droplet size bins for the sodium spray fire model. Remaining sodium was transferred to the sodium pool that collected onto the personal platform. It should be noted, that any aerosols entering the height of the pool mass region, no matter the insignificant amount of pool mass that exists, will be removed from a settled volume onto a heat structure. This was determined to be a mechanism for removing any settled masses from the bottom head and internal components. To maintain a similar comparison to that done previously by [3], the settled mass between the bottom head and internal components encompass a 50/50 split between aerosols that were found to be settled in the 'pool' volume through the plot parameter 'RN1-TYCLLIQ'.

The plated masses in the experiment also detailed different results when compared to the masses determined computationally. This may be attributed to the wash / sampling methods used to collect the masses, adding weight as a result of not being completely dried out. Assuming the same wash methods used for aerosol deposition, it is suspected that mass was added to the final mass determined for aerosol deposition as in test AB5/AB6 leading to an excess mass of up to 10% [14]. Despite the concerns with collected masses, our results still prove within error of experimental data.

3.1.1.4. Suspended Aerosol Concentration in Atmosphere

Two separate plots are shown in Figure 3-1 detailing the suspended aerosols of NaI and NaOH. The plot parameter 'RN1-TYCLAIR' was called for the NAC-enabled simulation to plot the airborne mass of a defined class (i.e. aerosol species) while existing data from the Souto model (1.8.6) used the 'RN1-ATRG' to plot the total radioactive aerosol in the gas phase.

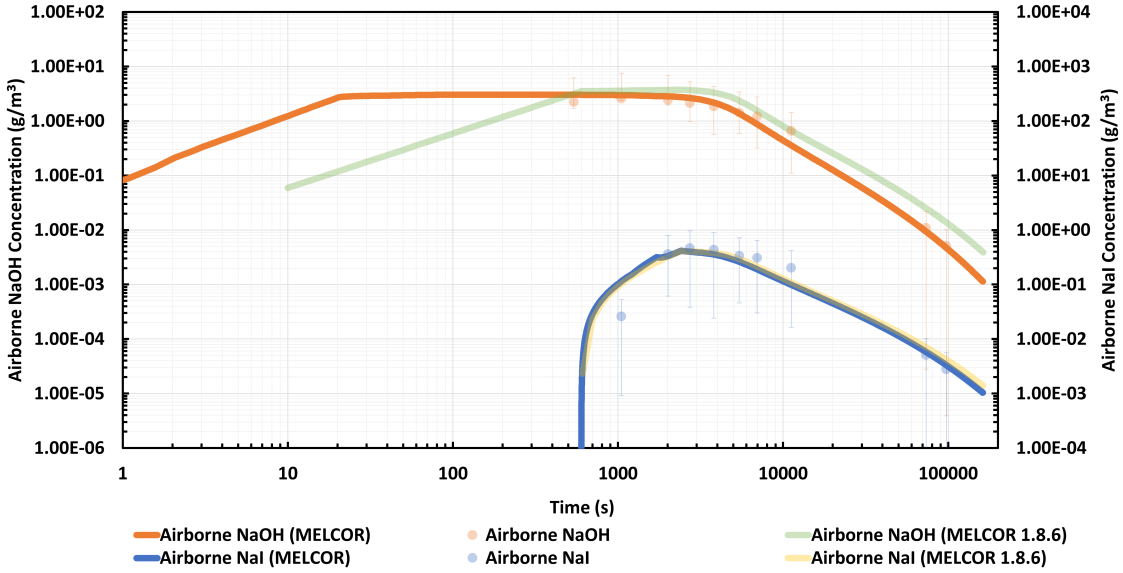

Figure 3-1. Suspended aerosol plots for the AB7 test.

As discussed in the previous iteration of this report [14], MELCOR is not able to accommodate the modeling of more than one aerosol's parameters (RN1_ASP) and thus cannot effectively address any stark differences between modeling a NaI aerosol, whose density was listed as 3670 kg m^{-1} vs. a NaOH aerosol, whose density was reported out to be 2130 kg m^{-1} (see 1-2). In addition to the differences in density, the aerosol agglomeration behavior cannot be adequately modeled per aerosol given differences in CHI, GAMMA, STICK, or TURBDS parameters for the aerosol physics. The previous report showcased some sensitivity perturbations applied to these key aerosol parameters which found that they greatly control the suspended aerosol levels [14].

3.1.2. Energy Generation & Dissipation

The NAC package in MELCOR controls all the atmospheric chemistry and pool fire reactions that would create/distribute energy to the system through Na combustion. An approximation had to be made for the use of the NAC_SPRAY field since there was no real spray event in this scenario, rather, it was a spill from a 11 mm diameter pipe. This pipe spilled toward an I-beam which then subsequently dripped the Na spill material down 10m to the personnel platform. The DME entry of the NAC_SPRAY field was used to control the amount of Na that combusted to form NaOH. The velocity of the spray was set to zero since it was assumed this material was dripping from the height specified. The atmospheric chemistry was controlled with the NAC_ATMCH field where all reactions were set to form NaOH, per the AB7 test report [12].

3.1.2.1. Combustion Mechanisms

To determine the amount of energy to add to the system, Souto's analysis relied on the calculation of the energy released during the following chemical reaction found in Eq 3.1. The total energy released from this reaction is as follows:

$$Q_1 = \left(\frac{6.434 \times 10^3 g}{2 \cdot (22.99 \frac{g}{mol})}\right) \cdot \left(85 \frac{kcal}{mol}\right) \cdot \left(4.184 \times 10^3 \frac{J}{kcal}\right) \tag{3.2}$$

Souto calculated that at total of 5.45E7J (54.5MJ) of combustion+residual energies were added into the atmosphere from the combustion of NaOH. The NAC-enabled simulation yielded a total energy added to the atmosphere of 1.56E7J (15.6MJ) and 0.423E7J (4.23MJ) added to the pool fire, yielding a combined total of 19.83MJ. Souto's calculation is an overestimation because test AB7 details that only about 2.92 kg of NaOH was produced. Thus, all of the Na could not have been combusted. Taking a proportionate fraction of Souto's estimation would yield 2.47E7J (24.7MJ), a value much more comparable to the results found in the NAC-enabled simulation and, if scaled down to our mass yield, would likely be equivalent.

3.1.2.2. Thermal-hydraulic Response

Figure 3-2 below compares the temperature and pressure plots between the original AB7 MELCOR 1.8.2 simulation (converted to 1.8.6), the NAC-enabled simulation using MELCOR 2.2, and the experimental test data.

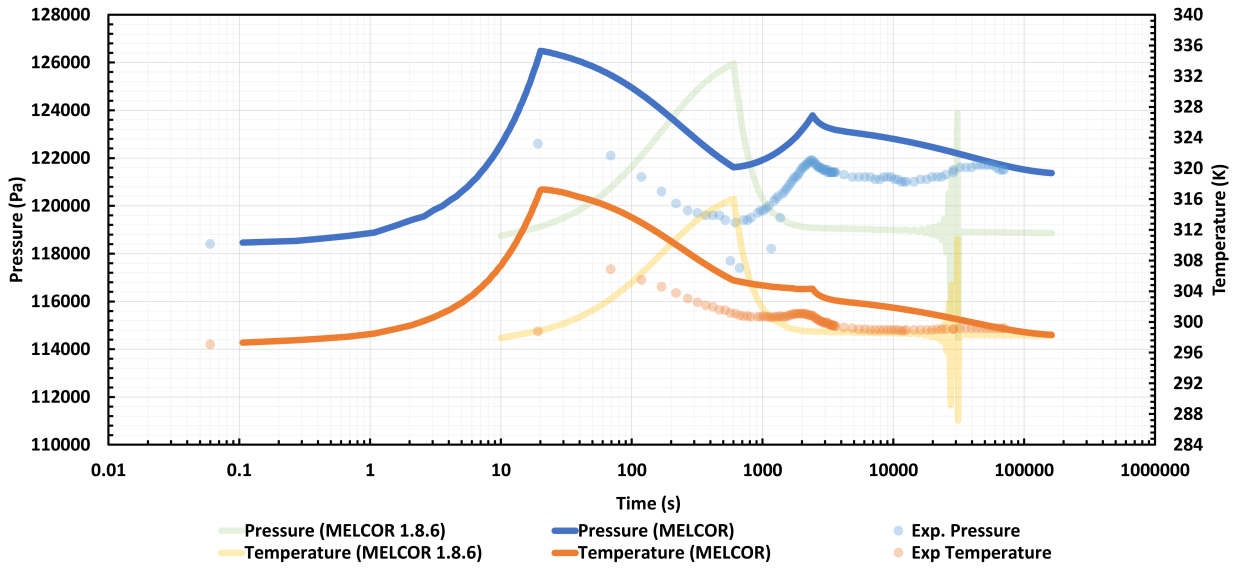

Figure 3-2. Pressure/Temperature plots for the AB7 test.

There is excellent agreement in the series of events that occur for this experiment and how they affect both the temperature and pressure responses within the new MELCOR simulations. The

only source of energy for Souto's analysis was that of the pool fire, hence, the curve that was generated is not representative of the actual experimental data. The initial spill was not considered effective in the Souto simulation resulting in an under approximation for the amount of energy deposited in the atmosphere in the first 20s. Souto's analysis did not account for the combustion that would occur from this spill as the leaked Na was falling a distance of 10m. This value is far greater than the fall height of the previous AB5/AB6 tests which was on the order of about 5m. Thus, the initial spike in the first 20s can solely be attributed to combustion of Na droplets in the CSTF atmosphere as they fall to the personnel platform. Then we have the burning pool fire (with area 0.92 m^2) which lasts from 20s to 600s. This is accurately captured in the NAC-enabled simulation, albeit a bit of an overestimation in both pressure and temperature of the containment atmosphere.

The overestimation is attributed to two possible causes: energy losses from the Na spill onto the I-beam support structure (as noted in [12]) and the lack of energy transfer from the fire directly to heat structures. Currently, MELCOR does not have a model to account for this phenomena but it is very likely that it will be implemented shortly after this work. And lastly, the final feature of the experimental data consists of a steady rise in pressure and temperature which is attributed to the injection of the NaI aerosol with its heated N_2 carrier gas. Since [12] did not reference a total amount of N_2 carrier gas injected into the system (did however note a temperature), the value was extrapolated from [1] data based on the NaI injection rate. The N_2 gas was assumed proportionate to the NaI injection rate.

For comparison of scale to the previous ABCOVE tests, AB5/AB6, we present, in Figure 3-3, the same data as in Figure 3-2, with y-axes scaling to match that of test AB6 results [14]. From this plot comparison, the magnitude and scale of the Na energy released to the atmosphere can be better viewed. What we are modeling for test AB7 is negligible for the effects and responses that occur in test AB6. In our attempt to model this extremely mild Na spill event, we are approaching sensitivities to previously negligible phenomenon. We are able to see, in the AB7 data, the effects of adding in some N_2 carrier gas whereas, for test AB6, it is completely overshadowed by the Na spray event. The bump in pressure observed in Figure 3-2 is on the order of about 4000 Pa or 4 kPa. That value equates to one tick gap in the pressure axes of Figure 3-3. The vast difference in energy imparted to the atmosphere when comparing test AB6 and AB7 is night and day. This comparison would be even greater of a difference if it was against test AB5, whose combustion event was much more violent and across a shorter time span.

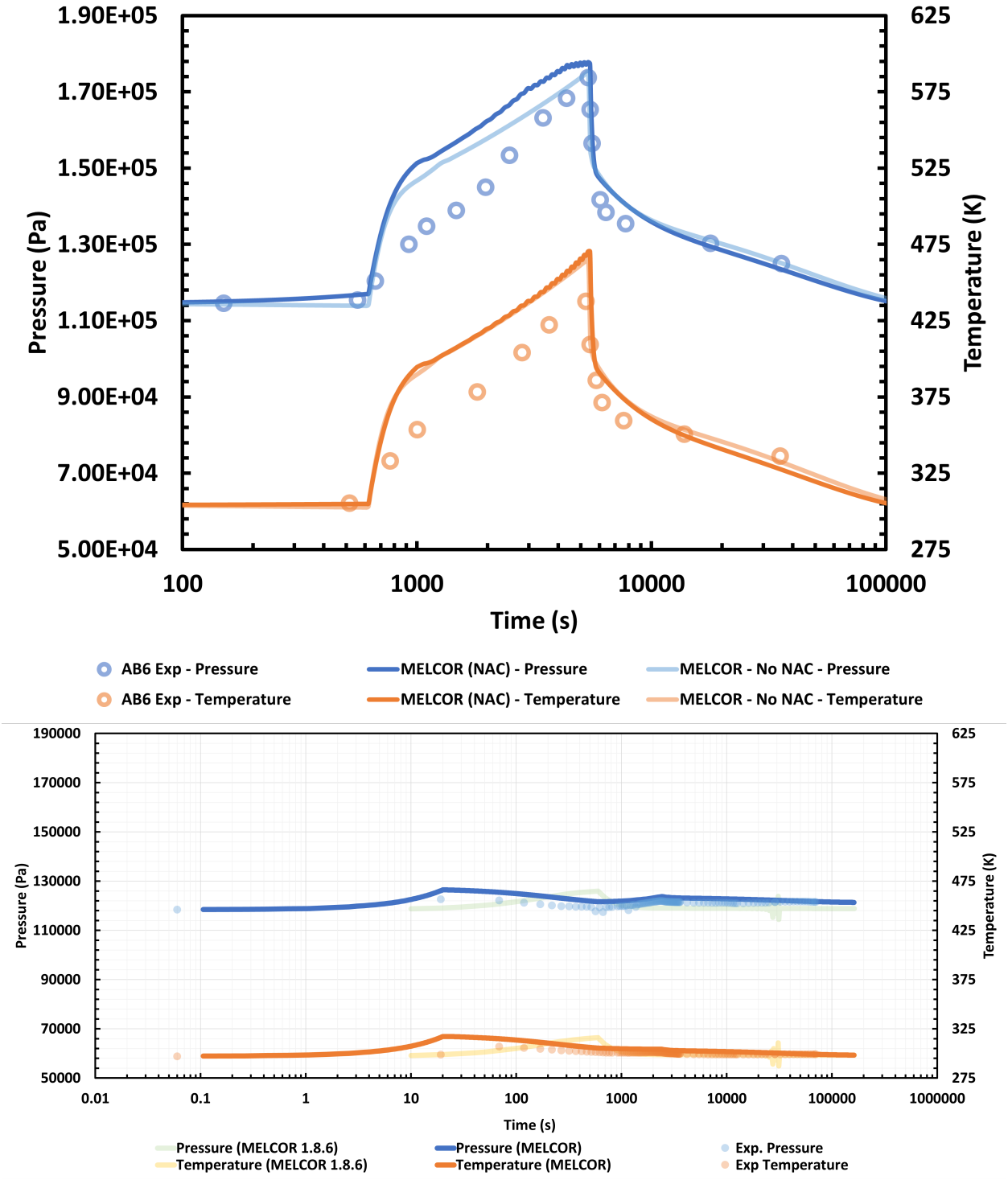

Figure 3-3. Pressure/Temperature plots for the AB6 (top [14]) and AB7 (bottom) tests.

4. CONCLUSION

The results of the AB7 test simulation using the NAC package showcased in this report serve to complete the reanalysis of the ABCOVE test series with modernized MELCOR methodologies for Na combustion modeling. This report, along with [14], should now provide the new benchmarks for the ABCOVE test series using MELCOR's NAC package in lieu of the original Souto analysis [3]. Despite the very mild conditions for Na combustion events, these new MELCOR simulations were able to capture the subtle changes and effects utilizing the NAC package's spray and pool fire models.

The analysis of test AB7 has provided significant insights into the aerosol and energy generation characteristics of sodium combustion. The comparison with a previous MELCOR assessment and experimental results highlights the importance of accurately modeling combustion events and aerosol behavior as well as capturing subtle experimental phenomena. Further knowledge of experimental intricacies, such as the amount of flow of Na onto the I-beam, would have improved this model's thermal-hydraulic response due to the deposition of heat onto the surface.

The findings indicate that the NAC package offers a more nuanced understanding of the in situ generation of Na aerosols and the associated thermal-hydraulic responses. Future efforts will require the incorporation of the energy transfer of combustion flames directly to heat structures to further improve the thermal-hydraulic of the NAC package. This brief study underscores the necessity of refining modeling techniques to account for the complexities of aerosol dynamics and energy transfer mechanisms in sodium-related incidents.

4.1. Lessons Learned

- **Incomplete Combustion of a Na Spill:** The analysis revealed that not all sodium combusted, leading to the formation of a sodium pool, which significantly affects the overall energy calculations and aerosol production.
- **Impact of Environmental Factors:** The presence of moisture in the atmosphere was identified as a limiting factor in the production of NaOH, emphasizing the need to consider environmental conditions in modeling.
- **Combustion Dynamics:** The study highlighted the underestimation of pressure and temperature effects due to incomplete combustion modeling, suggesting that future analyses should incorporate more detailed combustion dynamics such as flame to heat structure energy transfer.

- **Aerosol Behavior:** The differences in aerosol deposition and suspension behavior between NaOH and NaI necessitate tailored modeling approaches for different aerosol species to improve predictive accuracy. MELCOR is currently only capable of defining parameters for a single aerosol species which can hinder the transport and deposition characteristics if you have multiple species that are very different.
- **Thermal-Hydraulic Response:** The findings revealed a deficiency in MELCOR's current modeling capabilities when trying to capture the complexities of combustion flame heat transfer from flame to a heat structure. This was determined to lead to overestimations in thermal-hydraulic responses as it currently deposits all the energy to the atmosphere, highlighting a need for improvement.
- **Energy Generation and Dissipation:** The NAC-enabled simulation showed a more accurate representation of energy contributions from both the initial Na spill and the subsequent pool fire (when compared to the previous study [3]), highlighting the need to consider all energy sources in simulations.
- **Comparison with Previous Tests:** The analysis of pressure and temperature responses in test AB7 compared to AB6 illustrates the significant differences in energy release and thermal-hydraulic responses, emphasizing the need for all forms of pressure and temperature sources in modeling mild spill events as they become more noticeable in effects.

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APPENDIX A. AB7 Input Decks

A.1. MELCOR 1.8.6

```
*m: SNAP:Symbolic Nuclear Analysis Package, Version 4.3.0, May 17, 2024
*m: PLUGIN:MELCOR Version 2.8.8
*m: CODE:MELCOR Version 1.8.6
*m: DATE:10/8/24
*eor*      melgen
*
************************************************
TITLE 'Sensitivity test AB7.11'
************************************************
*
*:MODEL_OPTIONS
allowreplace
diagf llmlgAB7.dia
outputf llmlgAB7.out
pLotf llpltAB7.fil
restartf llpltAB7.rst
jobid llpltAB7
*
*********************************************
*       Writing out Tabular Functions       *
*********************************************
*
*
*d: EXTHEAT
*                  tfname        ntfpar        tfscal        tfadcn
TF00200            'TF_2'             4           1.0           0.0
*             ntfbdl        ntfbdu
TF00201            0             0
*   function data pairs
TF00210          0.0           0.0
TF00211          1.0        336.42
TF00212        600.0        4.98E7
TF00213       1.62E5        5.45E7
*
*d: ASOURCEL
*                  tfname        ntfpar        tfscal        tfadcn
TF00500            'TF_5'             3           1.0           0.0
*             ntfbdl        ntfbdu
TF00501            0             0
*   function data pairs
TF00510          0.0           1.0
TF00511        600.0           1.0
TF00512        601.0           0.0
*
*d: ASOURCE2
*                  tfname        ntfpar        tfscal        tfadcn
TF00600            'TF_6'             5           1.0           0.0
*             ntfbdl        ntfbdu
TF00601            0             0
*   function data pairs
TF00610          0.0           0.0
TF00611        599.0           0.0
TF00612        600.0           1.0
TF00613       2399.0           1.0
```

```
TF00614        2400.0           0.0
*
*d: DECAY
*                   tfname        ntfpar        tfscal        tfadcn
TF01000            'TF_10'             2           1.0           0.0
*              ntfbdl        ntfbdu
TF01001             0             0
*   function data pairs
TF01010           0.0           0.0
TF01011        1.62E5           0.0
*
*d: CPS-F
*                   tfname        ntfpar        tfscal        tfadcn
TF01100            'TF_11'             1           1.0           0.0
*              ntfbdl        ntfbdu
TF01101             0             0
*   function data pairs
TF01110           0.0         753.0
*
*d: THC-F
*                   tfname        ntfpar        tfscal        tfadcn
TF01200            'TF_12'             1           1.0           0.0
*              ntfbdl        ntfbdu
TF01201             0             0
*   function data pairs
TF01210           0.0        0.0467
*
*d: RHO-F
*                   tfname        ntfpar        tfscal        tfadcn
TF01300            'TF_13'             1           1.0           0.0
*              ntfbdl        ntfbdu
TF01301             0             0
*   function data pairs
TF01310           0.0          96.0
*
*d: CSTF-TEMP
*                   tfname        ntfpar        tfscal        tfadcn
TF20100           'TF_201'             2           1.0           0.0
*              ntfbdl        ntfbdu
TF20101             0             0
*   function data pairs
TF20110           0.0        298.15
TF20111        1.62E5        298.15
*
*****************************************
*       Writing out Materials (MP)        *
*****************************************
*
*
*                          matnam
MPMAT00000            'fiberglass'
*               prop    itbprp
MPMAT00001     'CPS'        11
MPMAT00002     'THC'        12
MPMAT00003     'RHO'        13
*********************************************************
*       Writing out Noncondensable Gasses (NCG)        *
*********************************************************
*
*
*
*n: N2
*              mname       mnumber
NCG000           N2             4
*
*n: O2
*              mname       mnumber
NCG001           O2             5
```

```
*
* bad - copied/pasted jp additions to ab6 to here since they are the same input records
*jp xxxxxx newly required record.  Indifferent to value.
DCHOPERPOW 1.0e1
DCHFPOW 0.0E0
*                wctype
DCHDECPOW         TF-10
*                                  rdcnam
DCHCLS0160                           'NAI'
*          clselm
DCHCLS0161   'LI'
DCHCLS0162   'NA'
DCHCLS0163    'K'
DCHCLS0164   'RB'
DCHCLS0165   'CS'
DCHCLS0166   'CU'
*                defcls
DCHDEFCLS0          ALL
*
*
*
************************************************
*       Writing out Control Volumes (CVH)        *
************************************************
*
*
*d: CSTF
*                  cvname        icvthr         icvff        icvtyp
CV00100            'CVH_1'             1             0             2
*               ipfsw        icvact
CV00101             0             0
*              itypth
CV001A0             3
* Thermodynamic input
CV001A1          PVOL       1.184E5
CV001A2          TATM        297.05
CV001A3          TDEW        274.65
CV001A4        MLFR.4        0.7905
CV001A5        MLFR.5        0.2095
* Altitude/volume table
CV001B0           0.0           0.0
CV001B1           1.9          50.0
CV001B2          18.4         752.0
CV001B3          20.3         852.0
* External Mass and Energy Sources
CV001C1            AE             2            0
*
*d: ENV
*                  cvname        icvthr         icvff        icvtyp
CV00200            'CVH_2'             1             0             6
*               ipfsw        icvact
CV00201             0             0
*              itypth
CV002A0             3
* Thermodynamic input
CV002A1          PVOL        1.01E5
CV002A2          TATM        298.15
CV002A3          VPOL           0.0
CV002A4        MLFR.4          0.79
CV002A5        MLFR.5          0.21
* Altitude/volume table
CV002B0           0.0           0.0
CV002B1        1.0E10        1.0E10
*
*
************************************************
*       Writing out Heat Structures (HS)        *
************************************************
```

```
*
*
*d: top head
*                    np         igeom           iss
HS00001000            7             1            -1
*                    hsname
HS00001001 'HS_1'
*                  hsalt         alpha
HS00001002          18.4           0.0
*                 nodloc        ifrmat            xi
HS00001100            -1             1           0.0
*                 xvalue        nxvalu
HS00001101        0.0193             2
HS00001102        0.0335             7
*                 mcdloc
HS00001200            -1
*                   matnam mshnum
HS00001201  STAINLESS-STEEL      1
HS00001202     'fiberglass'      6
*                   isrc
HS00001300            0
*           ibcl ibvl iflowl cpfpl cpfal
HS00001400     1    1    EXT   1.0   1.0
*                 emiswl         rmodl         pathl
HS00001401           0.9    GRAY-GAS-A          20.3
*                 asurfl          clnl         bndzl
HS00001500           63.0          7.62          7.62
*                   ibcr
HS00001600           2201
*                 ntdloc
HS00001800            -1
*                  tempin        nodnum
HS00001801         298.15             2
HS00001802         298.15             7
*
*d: walls-edge
*                    np         igeom           iss
HS00002000            7             2            -1
*                    hsname
HS00002001 'HS_2'
*                  hsalt         alpha
HS00002002           1.9           1.0
*                 nodloc        ifrmat            xi
HS00002100            -1             1          3.81
*                 xvalue        nxvalu
HS00002101        3.8269             2
HS00002102        3.8523             7
*                 mcdloc
HS00002200            -1
*                   matnam mshnum
HS00002201  STAINLESS-STEEL      1
HS00002202     'fiberglass'      6
*                   isrc
HS00002300            0
*           ibcl ibvl iflowl cpfpl cpfal
HS00002400     1    1    EXT   1.0   1.0
*                 emiswl         rmodl         pathl
HS00002401           0.9    GRAY-GAS-A          7.62
*                 asurfl          clnl         bndzl
HS00002500         394.0          7.62          16.5
*                   ibcr
HS00002600          2201
*                 ntdloc
HS00002800            -1
*                  tempin        nodnum
HS00002801         298.15             2
HS00002802         298.15             7
*
```

```
*d: vert-int
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*                    hsname
HS00003001 'HS_3'
*                  hsalt         alpha
HS00003002           0.0           1.0
*                 nodloc        ifrmat            xi
HS00003100           -1             1           0.0
*                 xvalue        nxvalu
HS00003101        8.4E-3             2
*                 mcdloc
HS00003200           -1
*                  matnam mshnum
HS00003201  STAINLESS-STEEL      1
*                  isrc
HS00003300           0
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HS00003400     1    1    EXT   1.0   1.0
*                 emiswl         rmodl         pathl
HS00003401           0.9    GRAY-GAS-A          3.81
*                 asurfl          clnl         bndzl
HS00003500         232.0          7.62          7.62
*           ibcr ibvr iflowr cpfpr cpfar
HS00003600     1    1    EXT   1.0   1.0
*                 emiswr         rmodr         pathr
HS00003601           0.9    GRAY-GAS-A          3.81
*                 asurfr          clnr         bndzr
HS00003700         232.0           7.0          0.62
*                 ntdloc
HS00003800           -1
*                  tempin        nodnum
HS00003801         297.05             2
*
*d: floor
*                    np         igeom           iss
HS00004000            7             1            -1
*                    hsname
HS00004001 'HS_4'
*                  hsalt         alpha
HS00004002        0.0435       -1.0E-7
*                 nodloc        ifrmat            xi
HS00004100           -1             1           0.0
*                 xvalue        nxvalu
HS00004101        0.0193             2
HS00004102        0.0447             7
*                 mcdloc
HS00004200           -1
*                  matnam mshnum
HS00004201  STAINLESS-STEEL      1
HS00004202     'fiberglass'      6
*                  isrc
HS00004300           0
*           ibcl ibvl iflowl cpfpl cpfal
HS00004400     1    1    EXT   1.0   1.0
*                 emiswl         rmodl         pathl
HS00004401           0.9    GRAY-GAS-A          20.3
*                 asurfl          clnl         bndzl
HS00004500        45.604          7.62          7.62
*                   ibcr
HS00004600          2201
*                 ntdloc
HS00004800           -1
*                  tempin        nodnum
HS00004801         298.15             2
HS00004802         298.15             7
*
*d: horz-int
```

```
*                    np         igeom           iss
HS00005000            2             1            -1
*                   hsname
HS00005001 'HS_5'
*                  hsalt         alpha
HS00005002           1.9           0.0
*                 nodloc        ifrmat            xi
HS00005100           -1             1           0.0
*                 xvalue        nxvalu
HS00005101        8.4E-3             2
*                 mcdloc
HS00005200           -1
*                  matnam mshnum
HS00005201  STAINLESS-STEEL      1
*                   isrc
HS00005300            0
*           ibcl ibvl iflowl cpfpl cpfal
HS00005400     1    1    EXT   1.0   1.0
*                 emiswl         rmodl         pathl
HS00005401           0.9    GRAY-GAS-A          3.81
*                 asurfl          clnl         bndzl
HS00005500        42.596           7.0          0.62
*           ibcr ibvr iflowr cpfpr cpfar
HS00005600     1    1    EXT   1.0   1.0
*                 emiswr         rmodr         pathr
HS00005601           0.9    GRAY-GAS-A          3.81
*                 asurfr          clnr         bndzr
HS00005700        42.596          7.62          7.62
*                 ntdloc
HS00005800           -1
*                  tempin        nodnum
HS00005801         297.05             2
*
*
* CORE PACKAGE DISABLED.
*
*              iactv
RN1000             0
*       numsec numcmp numcls nclsw nclsbx numsra numsrv nclcsi numca
RN1001      20      2     16    14     13      2      0     16     6
*                nclcs
RNCLS0000            2
*               nclsdn         xmrat
RNCLS0001            2           1.0
*              dmin          dmax        rhonom
RN1100        1.0E-7        1.0E-4        3670.0
*              icoeff
RNACOEF              1
*              pgas1         pgas2         tgas1         tgas2
RNPT000         1.0E5         1.5E5         290.0         308.0
*                chi         gamma         fslip         stick
RNMS000          1.5          2.25          1.37           1.0
*              turbds         tkgop        ftherm        deldif
RNMS001        1.0E-3          0.05           1.0        1.0E-5
*        ix1 ix2 ix3 ix4 ix5 ix6 ix7 ix8 ix9 ix10 ix11 ix12 ix13 ix14 ix15 ix16 ix17
RNCC000    1   1   1   1   1   1   1   1   1    1    1    1    1    1    1    2   -1
*                 ids          isde          ityp
RNDS000             1           LHS       CEILING
RNDS001             2           LHS          WALL
RNDS002             3           LHS          WALL
RNDS003             4           LHS         FLOOR
RNDS004             5           LHS         FLOOR
RNDS005             3           RHS      INACTIVE
RNDS006             5           RHS      INACTIVE
*               ivolf         ivolt          elev          area
RNSET000             2             2           0.0           1.0
*        ivol iphs iclss rfrs      xm itab idist
RNAS000     1    2     2  0.0 5.03E-3    5     2
```

```
*                geomm           gsd
RNAS001         5.0E-7           2.0
*        ivol iphs iclss rfrs      xm itab idist
RNAS002     1    2    16  1.0 1.97E-4    6     2
*                geomm           gsd
RNAS003         5.4E-7          1.55

.
*eor* melcor
************************************************
TITLE 'Sensitivity test AB7.1 l'
************************************************
*
*
DTTIME 10.0
*
diagf llmlcAB7.dia
messagef llmlcAB7.mes
outputf llmlcAB7.out
pLotf llpltAB7.fil
restartf llpltAB7.rst
jobid llpltAB7
*
RESTART -1
*
TIME1           0.0          10.0         0.01       10000.0          10.0       50000.0        1.0E10
TIME2          10.0          10.0         0.01       10000.0          10.0       50000.0        1.0E10
TIME3          30.0          10.0         0.01       10000.0          10.0       50000.0        1.0E10
TIME4          60.0          10.0         0.01       10000.0          40.0       50000.0        1.0E10
TIME5         300.0          10.0         0.01       10000.0          50.0       50000.0        1.0E10
TIME6         600.0          10.0         0.01       10000.0         100.0       50000.0        1.0E10
TIME7        1200.0          10.0         0.01       12000.0         400.0       50000.0        1.0E10
TIME8        2400.0        1000.0         0.01       12000.0         400.0       50000.0        1.0E10
*
TEND 5.4321E20
.
```

A.2. MELCOR 2.2

```
!******************************************************************************
!******************************************************************************
! $Id$
! Abcove AB7
! Sensitivity case: 20 sections aerosol bin
!
! Developed by:
! Sandia National Laboratories
!******************************************************************************

MEG_DIAGFILE 'AB7G.DIA'
MEG_OUTPUTFILE 'AB7G.OUT'
MEG_RESTARTFILE 'AB7G.RST'
MEL_DIAGFILE 'AB7.DIA'
MEL_OUTPUTFILE 'AB7.OUT'
MEL_RESTARTFILE 'AB7G.RST'  -1
PLOTFILE 'AB7.PTF'
MESSAGEFILE 'AB7.MES'
NOTEPAD++ ON
READFLUID 'SIMMER'



program melgen

!block: 'melgenbase'

EXEC_INPUT !(
EXEC_TITLE 'Sensitivity test AB7'
EXEC_DTTIME 1.0E-3
EXEC_GLOBAL_DFT 2.0  ! global flag for 2.0 is used.
EXEC_JOBID 'REF'
EXEC_PLOT   53 !(
    1  RN1-TYCLAIR(CS,'CTYP-2','TOT')
    2  RN1-TYCLAIR(NAI,'CTYP-2','TOT')
    3  RN1-TYCLAIR(NA2O2,'CTYP-2','TOT')
    4  RN1-TYCLAIR(NAOH,'CTYP-2','TOT')
    5  RN1-ADEP('top head',LHS,'CS',TOT)
    6  RN1-ADEP('walls-edge_lower',LHS,'CS',TOT)
    7  RN1-ADEP('walls-edge_upper',LHS,'CS',TOT)
    8  RN1-ADEP('vert-int',LHS,'CS',TOT)
    9  RN1-ADEP('floor',LHS,'CS',TOT)
    10 RN1-ADEP('pplatform',LHS,'CS',TOT)
    11 RN1-ADEP('horiz-int',LHS,'CS',TOT)
    12 RN1-ADEP('top head',LHS,'NAI',TOT)
    13 RN1-ADEP('walls-edge_lower',LHS,'NAI',TOT)
    14 RN1-ADEP('walls-edge_upper',LHS,'NAI',TOT)
    15 RN1-ADEP('vert-int',LHS,'NAI',TOT)
    16 RN1-ADEP('floor',LHS,'NAI',TOT)
    17 RN1-ADEP('pplatform',LHS,'NAI',TOT)
    18 RN1-ADEP('horiz-int',LHS,'NAI',TOT)
    19 RN1-ADEP('top head',LHS,'NA2O2',TOT)
    20 RN1-ADEP('walls-edge_lower',LHS,'NA2O2',TOT)
    21 RN1-ADEP('walls-edge_upper',LHS,'NA2O2',TOT)
    22 RN1-ADEP('vert-int',LHS,'NA2O2',TOT)
    23 RN1-ADEP('floor',LHS,'NA2O2',TOT)
    24 RN1-ADEP('pplatform',LHS,'NA2O2',TOT)
    25 RN1-ADEP('horiz-int',LHS,'NA2O2',TOT)
    26 RN1-VDEP('top head',LHS,'NA2O2',TOT)
    27 RN1-VDEP('walls-edge_lower',LHS,'NA2O2',TOT)
    28 RN1-VDEP('walls-edge_upper',LHS,'NA2O2',TOT)
    29 RN1-VDEP('vert-int',LHS,'NA2O2',TOT)
    30 RN1-VDEP('floor',LHS,'NA2O2',TOT)
    31 RN1-VDEP('pplatform',LHS,'NA2O2',TOT)
    32 RN1-VDEP('horiz-int',LHS,'NA2O2',TOT)
```

```
    33 RN1-ADEP('top head',LHS,'NAOH',TOT)
    34 RN1-ADEP('walls-edge_lower',LHS,'NAOH',TOT)
    35 RN1-ADEP('walls-edge_upper',LHS,'NAOH',TOT)
    36 RN1-ADEP('vert-int',LHS,'NAOH',TOT)
    37 RN1-ADEP('floor',LHS,'NAOH',TOT)
    38 RN1-ADEP('pplatform',LHS,'NAOH',TOT)
    39 RN1-ADEP('horiz-int',LHS,'NAOH',TOT)
    40 RN1-VDEP('top head',LHS,'NAOH',TOT)
    41 RN1-VDEP('walls-edge_lower',LHS,'NAOH',TOT)
    42 RN1-VDEP('walls-edge_upper',LHS,'NAOH',TOT)
    43 RN1-VDEP('vert-int',LHS,'NAOH',TOT)
    44 RN1-VDEP('floor',LHS,'NAOH',TOT)
    45 RN1-VDEP('pplatform',LHS,'NAOH',TOT)
    46 RN1-VDEP('horiz-int',LHS,'NAOH',TOT)
    47 RN1-VDEP('top head',LHS,'NAI',TOT)
    48 RN1-VDEP('walls-edge_lower',LHS,'NAI',TOT)
    49 RN1-VDEP('walls-edge_upper',LHS,'NAI',TOT)
    50 RN1-VDEP('vert-int',LHS,'NAI',TOT)
    51 RN1-VDEP('floor',LHS,'NAI',TOT)
    52 RN1-VDEP('pplatform',LHS,'NAI',TOT)
    53 RN1-VDEP('horiz-int',LHS,'NAI',TOT)

!eos_input


! EOS_FLUID_ID "sodium" 1
! EOS_FLUID_TYPE tpf Na "tpfna"
!
!
! EOS_NETWORK_ID "ABCOVE AB7" 12
! EOS_NETWORK_CV "CSTF_upper"
! EOS_NETWORK_FLUID "sodium"

TF_INPUT !(
TF_ID           'EXHEAT'           1.0           0.0 !(
TF_TAB    4 !n             x             y
            1           0.0           0.0
            2           1.0           0.0
            3         600.0        4.98e7
            4        1.62e5        5.45e7
!)
! N2 source feeding in with NaI
TF_ID         'N2SOURCE'           1.0           0.0 !(
TF_TAB    5 !n             x             y
            1           0.0           0.0
            2         599.0           0.0
            3         600.0           0.013767
            4        2400.0           0.013767
            5        2400.1           0.0
TF_ID         'N2TEMP'           1.0           0.0 !(
TF_TAB    5 !n             x             y
            1           0.0           0.0
            2         599.0           0.0
            3         600.0           428.15 ! changed to DAS#105 value, nucleator outlet temperature ~155C \ old 493.15 K
            4        2400.0           428.15 ! changed to DAS#105 value, nucleator outlet temperature ~155C \ old 493.15 K
            5        2400.1           0.0
TF_ID         'ASOURCE2'           1.0           0.0 !(
TF_TAB    6 !n             x             y
            1           0.0           0.0
            2         599.0           0.0
            3         600.0           1.0
            4        2400.0           1.0
            5        2400.1           0.0
            6        100000.0         0.0

TF_ID         'SPRAY-M'           1.0           0.0 !(
TF_TAB    5 !n             x             y
            1           0.0           0.322
```

```
            2          19.9           0.322
            3          20.0           0.0
            4         100.0           0.0
            5        1.62e5           0.0
TF_ID         'SPRAY-T'           1.0           0.0 !(
TF_TAB    5 !n             x             y
            1           0.0           863.15
            2          19.9           863.15
            3          20.0           0.0
            4         100.0           0.0
            5        1.62e5           0.0
TF_ID         'SPRAY-V'           1.0           0.0 !(
TF_TAB    5 !n             x             y
            1           0.0           0.0 !3.64
            2          19.9           0.0 !3.64
            3          20.0           0.0
            4         100.0           0.0
            5        1.62e5           0.0
!)
TF_ID            'DECAY'           1.0           0.0 !(
TF_TAB    2 !n             x             y
            1           0.0           0.0
            2        1.62e5           0.0
!)
TF_ID            'CPS-F'           1.0           0.0 !(
TF_TAB    2 !n             x             y
            1           0.0           0.0
            2           0.0          753.0
!)
TF_ID            'THC-F'           1.0           0.0 !(
TF_TAB    2 !n             x             y
            1           0.0           0.0
            2           0.0         0.0467
!)
TF_ID            'RHO-F'           1.0           0.0 !(
TF_TAB    2 !n             x             y
            1           0.0           0.0
            2           0.0          96.0
!)
TF_ID        'CSTF-TEMP'           1.0           0.0 !(
TF_TAB    2 !n             x             y
            1           0.0         298.15
            2        1.62e5         298.15
!)

!CF_INPUT


MP_INPUT !(
MP_ID              'fiberglass' !(
MP_PRTF    3 !n          prop        itbprp         cfkey
            1           CPS       'CPS-F'
            2           THC       'THC-F'            TF
            3           RHO       'RHO-F'
!)
MP_ID           CARBON-STEEL
!)

NCG_INPUT !(

NCG_ID        'N2'
NCG_ID        'O2'
NCG_ID        'H2OV'
NCG_ID    'H2'
!)

DCH_INPUT !(
DCH_RCT            PWR
```

```
DCH_SHT           TIME           0.0
DCH_OPW      0.0 !2.68597E9
DCH_DPW             TF       'DECAY'
DCH_FPW        0.0  0.0   0.0
!DCH_FPW       1.7387E9      8.3423E8      1.1304E8
! Define zero power decay heat tables for elements
! within the new Na Classes
DCH_EL N1    0.0  2
                    1   0.0    0.0
                    2   1.0E10 0.0
DCH_EL N2    0.0  2
                    1   0.0    0.0
                    2   1.0E10 0.0
DCH_EL N3    0.0  2
                    1   0.0    0.0
                    2   1.0E10 0.0
DCH_EL N4    0.0  2
                    1   0.0    0.0
                    2   1.0E10 0.0
DCH_EL N5    0.0  2
                    1   0.0    0.0
                    2   1.0E10 0.0
!DCH Classes
!(
DCH_CL  'XE'   DEFAULT  ! 1
DCH_CL  'CS'   DEFAULT  ! 2
DCH_CL  'BA'   DEFAULT  ! 3
DCH_CL  'I2'   DEFAULT  ! 4
DCH_CL  'TE'   DEFAULT
DCH_CL  'RU'   DEFAULT
DCH_CL  'MO'   DEFAULT
DCH_CL  'CE'   DEFAULT
DCH_CL  'LA'   DEFAULT
DCH_CL  'UO2'   DEFAULT
DCH_CL  'CD'   DEFAULT
DCH_CL  'AG'   DEFAULT
DCH_CL  'BO2'   DEFAULT
DCH_CL  'NA'   DEFAULT
DCH_CL  'CON'   DEFAULT
DCH_CL  'CSI'   DEFAULT
DCH_CL  'CSM'   DEFAULT
DCH_CL  'H2OA'  USER 1
                    1  'N1'
DCH_CL  'NAOH'  USER 1
                    1  'N2'
DCH_CL  'NA2O2' USER 1
                    1  'N3'
DCH_CL  'NA2O'  USER 1
                    1  'N4'
DCH_CL  'NAI'  USER 1
                    1  'N5'
!)

CVH_INPUT !(
!
! CSTF - containment vessel
! Env  - environment volume
!
CV_ID        'CSTF_lower'             1 !(
CV_TYP       'CTYP-2'
CV_THR       NONEQUIL           FOG         ACTIVE
CV_PAS       SEPARATE       ONLYATM   SUPERHEATED
CV_PTD           PVOL       1.184e5
CV_AAD           TATM        297.05
!cv_pas       separate poolandatm subcooled saturated
!cv_ptd       pvol            1.184e5     TATM 295.05
!cv_pad                       629.06
!cv_bnd       zpol            0.000
```

```
CV_NCG              4          RHUM          0.0
!                   n        namgas          mass
                    1          'N2'         0.7843 !0.7905  -  0.00688
                    2          'O2'         0.2095
     3          'H2OV'       0.0062
     4   'H2'  0.0000
! these vals are based off https://www.quadco.engineering/en/know-how/cfd-calculate-water-fraction-humid-air.htm
! and https://www.hanford.gov/files.cfm/Monthly_Average_Relative_Humidity.pdf data for humidity at 30 C on July 1983
!!!'N2'         0.76245
!!!'O2'         0.22774
!!!'H2OV'       0.00981
CV_VAT    3 !n           cvz         cvvol
            1           0.0           0.0
            2           1.9          50.0
   3    7.6   292.5
CV_SOU    2 !n          ctyp        interp        iessrc       idmat
   1   mass     rate       tf        'N2SOURCE'       N2
   2   te       rate       tf        'N2TEMP'         -1

CV_ID              'CSTF_upper'             2 !(
!CV_TYP           'CTYP-2'
!         NONEQUIL           FOG         ACTIVE
!CV_PAS       SEPARATE       ONLYATM   SUPERHEATED
!CV_PTD           PVOL       1.184e5
!CV_AAD           TATM        297.05
CV_TYP           'CTYP-3'
CV_THR         NONEQUIL           FOG         ACTIVE
cv_pas       SEPARATE    POOLANDATM     SUBCOOLED   SUPERHEATED
CV_PTD           PVOL       1.184e5
cv_pad          829.06
CV_AAD           TATM        297.05
cv_bnd       vpol            0.00076
CV_PDIA 1.088 ! exp determined pool area: 0.93 m^2

CV_NCG              4          RHUM          0.0
!                   n        namgas          mass
                    1          'N2'         0.7843 !0.7905  -  0.00688
                    2          'O2'         0.2095
     3          'H2OV'       0.0062
     4   'H2'  0.0000
CV_VAT    4 !n           cvz         cvvol
   1   7.6   0.0
   2   7.6018  0.0076
            3          18.4         459.4
            4          20.3         559.4

CV_ID              'ENV'             3 !(
CV_TYP           'CTYP-6'
!CV_THR         EQUIL           FOG         ACTIVE
CV_THR         EQUIL           FOG     TIME-INDEP
!CV_PAS       SEPARATE    POOLANDATM     SATURATED   SUPERHEATED
CV_PAS       SEPARATE       ONLYATM   SUPERHEATED
CV_PTD           PVOL        1.01E5
CV_AAD           TATM        298.15
CV_NCG              2          RHUM           0.0
!                   n        namgas          mass
                    1          'N2'          0.79
                    2          'O2'          0.21
!               bndid          vpol
!CV_BND           VPOL           0.0
CV_VAT    2 !n           cvz         cvvol
            1         0.0           0.0
            2        20.3          852.0
!)
!)
FL_INPUT
fl_id          'FL_1'             1
fl_ft     'CSTF_upper'  'CSTF_lower'         8.0   7.0
```

```
fl_geo       45.6  0.5      1.0     7.0   8.0
!fl_geo       22.8  0.5      1.0     7.0   8.0
fl_jsw 0 0 0
fl_vel 0.1 0.0
fl_usl         1.0E-5        1.0E-5           1.0           1.0
fl_seg    1 !n    sarea   slen     shyd srgh lamflg slam
!             1   22.8   0.4  3.81
            1   45.6   0.4  7.62

! fl_vtm ---input for transient mixing

fl_id          'FL_2'             2
fl_ft     'CSTF_lower'  'CSTF_upper'         7.0    8.0
fl_geo       45.6  0.5      1.0     7.0    8.0
!fl_geo       22.8  0.5      1.0     7.0   8.0
fl_jsw 0 0 0
fl_vel 0.1 0.0
fl_usl         1.0E-5        1.0E-5           1.0           1.0
fl_seg    1 !n    sarea   slen     shyd srgh lamflg slam
!             1   22.8   0.4  3.81
            1   45.6   0.4  7.62

HS_INPUT !(
!
! * There are 5 heat structures:
! * - 1 is the CSTF top head
! * - 2 are the CSTF cylindrical walls
! * - 3 represents the internal components for aerosol plating
! * - 4 is the CSTF bottom head
! * - 5 are the internal components for aerosol settling
!
! HS 1 = CSTF TOP HEAD
!
!              hsname        ishnum
HS_ID      'top head'             1 !(  63  x
!               igeom          iss
HS_GD     RECTANGULAR           NO
!              hsalt         alpha
HS_EOD          18.4           0.0
!              isrc
HS_SRC            NO
!      size
HS_ND     10 !n n      xi tempin          matnam
            1  1  0.00000 303.45 CARBON-STEEL
            2  2  0.00500 303.45 CARBON-STEEL
            3  3  0.01000 303.45 CARBON-STEEL
            4  4  0.01500 303.45 CARBON-STEEL
            5  5  0.01810 298.15    'fiberglass'
            6  6  0.02118 298.15    'fiberglass'
            7  7  0.02426 298.15    'fiberglass'
            8  8  0.02734 298.15    'fiberglass'
            9  9  0.03042 298.15    'fiberglass'
            10 10 0.03350 298.15
!              ibcl                       ibvl        mteval
HS_LB      CalcCoefHS                   'CSTF_upper'           YES
!              emiswl         rmodl         pathl
HS_LBR            0.9    GRAY-GAS-A          20.3
!              iflowl         cpfpl         cpfal
HS_LBP            EXT           1.0           1.0
!              asurfl          clnl         bndzl
HS_LBS          63.0          7.62          7.62
!               ibcr         table
HS_RB      TempTimeTF   'CSTF-TEMP'
!              iflowr         cpfpr         cpfar
HS_RBP            INT           0.0           0.0
!               iftnum
HS_FT             OFF
!)
```

```
! HS 2 upper = CSTF CYLINDER WALLS
!
!              hsname        ishnum
HS_ID    'walls-edge_lower'             2 !( 395
!               igeom           iss
HS_GD     CYLINDRICAL            NO
!               hsalt         alpha
HS_EOD            1.9           1.0
!               isrc
HS_SRC              NO
!      size
HS_ND     10 !n n      xi tempin          matnam
            1  1   3.81000 301.55 CARBON-STEEL
            2  2   3.81500 301.55 CARBON-STEEL
            3  3   3.82000 301.55 CARBON-STEEL
            4  4   3.82500 301.55 CARBON-STEEL
            5  5   3.83290 298.15    'fiberglass'
            6  6   3.83798 298.15    'fiberglass'
            7  7   3.84306 298.15    'fiberglass'
            8  8   3.84814 298.15    'fiberglass'
            9  9   3.85322 298.15    'fiberglass'
            10 10  3.85830 298.15
!               ibcl                        ibvl        mteval
HS_LB      CalcCoefHS                    'CSTF_lower'           YES
!              emiswl         rmodl         pathl
HS_LBR            0.9    GRAY-GAS-A          7.62
!              iflowl         cpfpl         cpfal
HS_LBP            EXT           1.0           1.0
!              asurfl          clnl         bndzl
HS_LBS           259.9          7.62          5.7
!               ibcr         table
HS_RB      TempTimeTF   'CSTF-TEMP'
!              iflowr         cpfpr         cpfar
HS_RBP            INT           0.0           0.0
!               iftnum
HS_FT              OFF
!)
! HS 2 upper = CSTF CYLINDER WALLS
!
!              hsname        ishnum
HS_ID    'walls-edge_upper'             3 !( 395
!               igeom           iss
HS_GD     CYLINDRICAL            NO
!               hsalt         alpha
HS_EOD            7.6           1.0
!               isrc
HS_SRC              NO
!      size
HS_ND     10 !n n      xi tempin          matnam
            1  1   3.81000 301.55 CARBON-STEEL
            2  2   3.81500 301.55 CARBON-STEEL
            3  3   3.82000 301.55 CARBON-STEEL
            4  4   3.82500 301.55 CARBON-STEEL
            5  5   3.83290 298.15    'fiberglass'
            6  6   3.83798 298.15    'fiberglass'
            7  7   3.84306 298.15    'fiberglass'
            8  8   3.84814 298.15    'fiberglass'
            9  9   3.85322 298.15    'fiberglass'
            10 10  3.85830 298.15
!               ibcl                        ibvl        mteval
HS_LB      CalcCoefHS                    'CSTF_upper'           YES
!              emiswl         rmodl         pathl
HS_LBR            0.9    GRAY-GAS-A          7.62
!              iflowl         cpfpl         cpfal
HS_LBP            EXT           1.0           1.0
!              asurfl          clnl         bndzl
HS_LBS           405.9          7.62          8.9
!               ibcr         table
```

```
HS_RB      TempTimeTF   'CSTF-TEMP'
!              iflowr         cpfpr         cpfar
HS_RBP            INT           0.0           0.0
!               iftnum
HS_FT              OFF
!)
! HS 3 = INTERNAL COMPONENTS FOR PLATING
!
!              hsname        ishnum
HS_ID      'vert-int'             4  !( 232  x
!               igeom          iss
HS_GD     RECTANGULAR           NO
!               hsalt        alpha
HS_EOD            0.0          1.0
!               isrc
HS_SRC            NO
!      size
HS_ND     3 !n n     xi tempin          matnam
            1 1    0.0 302.25 CARBON-STEEL
            2 2 1.4E-3 302.25 CARBON-STEEL
            3 3 3.4E-3 302.25
!               ibcl                        ibvl        mteval
HS_LB      CalcCoefHS                    'CSTF_lower'          YES
!              emiswl         rmodl         pathl
HS_LBR            0.9    GRAY-GAS-A          3.81
!              iflowl         cpfpl         cpfal
HS_LBP            EXT           1.0           1.0
!              asurfl         clnl          bndzl
HS_LBS          232.0          7.62          7.6 !7.62
!               ibcr                        ibvr        mteval
HS_RB      CalcCoefHS                    'CSTF_lower'          YES
!              emiswr         rmodr         pathr
HS_RBR            0.9    GRAY-GAS-A          3.81
!              iflowr         cpfpr         cpfar
HS_RBP            EXT           1.0           1.0
!              asurfr         clnr          bndzr
HS_RBS          232.0          7.62          7.6 !7.62
!               iftnum
HS_FT              OFF
!)
! HS 4 = BOTTOM HEAD
!
!              hsname        ishnum
HS_ID         'floor'             5 !( 45.6
!               igeom          iss
HS_GD     RECTANGULAR           NO
!               hsalt        alpha
!HS_EOD         -0.0435      -1.0E-7
HS_EOD         0.000       -1.0E-7   !!!!!!!!!!WARNING
!               isrc
HS_SRC            NO
!      size
HS_ND     10 !n n      xi tempin          matnam
            1  1  0.00000 301.55 CARBON-STEEL
            2  2  0.00400 301.55 CARBON-STEEL
            3  3  0.00800 301.55 CARBON-STEEL
            4  4  0.01200 301.55 CARBON-STEEL
            5  5  0.01810 298.15    'fiberglass'
            6  6  0.02318 298.15    'fiberglass'
            7  7  0.02826 298.15    'fiberglass'
            8  8  0.03334 298.15    'fiberglass'
            9  9  0.03842 298.15    'fiberglass'
            10 10 0.04350 298.15
!               ibcl                        ibvl        mteval
HS_LB      CalcCoefHS                    'CSTF_lower'          YES
!              emiswl         rmodl         pathl
HS_LBR            0.9    GRAY-GAS-A          20.3
!              iflowl         cpfpl         cpfal
```

```
HS_LBP            EXT           1.0           1.0
!              asurfl          clnl         bndzl
HS_LBS         45.604          7.62          7.6 !7.62
!                ibcr         table
HS_RB      TempTimeTF   'CSTF-TEMP'
!              iflowr         cpfpr         cpfar
HS_RBP            INT           0.0           0.0
!               iftnum
HS_FT              OFF
!)
! HS 5 = INTERNAL COMPONENTS FOR SETTLING
!
!              hsname        ishnum
HS_ID     'horiz-int'             6 !( 42.696  x
!               igeom          iss
HS_GD     RECTANGULAR           NO
!               hsalt         alpha
HS_EOD            1.9           0.0
!               isrc
HS_SRC              NO
!      size
HS_ND     3 !n n     xi tempin          matnam
            1 1    0.0 302.25 CARBON-STEEL
            2 2 1.4E-3 302.25 CARBON-STEEL
            3 3 3.4E-3 302.25
!               ibcl                         ibvl        mteval
HS_LB      CalcCoefHS                     'CSTF_lower'           YES
!              emiswl         rmodl         pathl
HS_LBR            0.9    GRAY-GAS-A          3.81
!              iflowl         cpfpl         cpfal
HS_LBP            EXT           1.0           1.0
!              asurfl          clnl         bndzl
HS_LBS         42.696          7.62          7.62
!                ibcr                         ibvr        mteval
HS_RB      CalcCoefHS                     'CSTF_lower'           YES
!              emiswr         rmodr         pathr
HS_RBR            0.9    GRAY-GAS-A          3.81
!              iflowr         cpfpr         cpfar
HS_RBP            EXT           1.0           1.0
!              asurfr          clnr         bndzr
HS_RBS         42.696          7.62          7.62
!                iftnum
HS_FT              OFF
!)
! HS 6 = Personnel Platform
!
!              hsname        ishnum
HS_ID     'pplatform'             7 !( 42.696  x
!               igeom          iss
HS_GD     RECTANGULAR           NO
!               hsalt         alpha
HS_EOD            7.6           0.0
!               isrc
HS_SRC              NO
!      size
HS_ND     3 !n n     xi tempin          matnam
            1 1    0.0 302.25 CARBON-STEEL
            2 2 1.4E-3 302.25 CARBON-STEEL
            3 3 3.4E-3 302.25
!               ibcl                         ibvl        mteval
HS_LB      CalcCoefHS                     'CSTF_lower'           YES
!              emiswl         rmodl         pathl
HS_LBR            0.9    GRAY-GAS-A          3.81
!              iflowl         cpfpl         cpfal
HS_LBP            EXT           1.0           1.0
!              asurfl          clnl         bndzl
HS_LBS         4.2          0.5          0.5
!                ibcr                         ibvr        mteval
```

```
HS_RB      CalcCoefHS                     'CSTF_upper'          YES
!              emiswr         rmodr         pathr
HS_RBR           0.9    GRAY-GAS-A          3.81
!              iflowr         cpfpr         cpfar
HS_RBP           EXT            1.0           1.0
!              asurfr          clnr         bndzr
HS_RBS         4.2          0.5          0.5
!               iftnum
HS_FT             OFF
!)
!)

RN1_INPUT             0 !(
!
!
RN1_DIM             20             3            22             6
RN1_DCHNORM          NONE
!
! ** AEROSOL PARAMETERS
! * 0.1e-6 = Lower bound for aersosol diameter
! * 100.0e-6 = Upper bound for aerosol diameter
! * 3670 = NaI density
! ********************************************************************
! * Note: MELCOR allows the inclusion of parameters (e.g.the density) for only one component.
! *      Since we are interested in plot the NaI component, we will use its density
! ********************************************************************
!
!                dmin          dmax        rhonom
! RN1_ASP       1.0E-7         1.0E-4         3670.0
RN1_ASP         1.0E-8         1.0e-4         3670.0
RN1_ACOEF      CALANDWR
RN1_PT        50000.0         2.0E6         270.0         1000.0
!                chi          gamma         fslip          stick
!RN1_MS00          1.5           2.25          1.37            1.0    ! from SAND94-2166
RN1_MS00          1.5           2.25          1.37            1.0
!              turbds          tkgop         ftherm        deldif
!RN1_MS01         1.0E-3          0.05           1.0        1.0E-5    ! from SAND94-2166
RN1_MS01         1.0000e-3        5.0000e-2       2.2500e+0     1.0000e-5
 RN1_DS    10 !n           ids          isde          ityp
            1    'top head'           LHS       CEILING
            2  'walls-edge_upper'     LHS          WALL
            3  'walls-edge_lower'     LHS          WALL
            4    'vert-int'           LHS          WALL
            5       'floor'           LHS         FLOOR
            6   'horiz-int'           LHS         FLOOR
            7    'vert-int'           RHS      INACTIVE
            8   'horiz-int'           RHS      INACTIVE
            9   'pplatform'           LHS       CEILING
            10   'pplatform'          RHS       FLOOR

RN1_SET    1 !n         ivolf         ivolt          elev          area
            1         'ENV'         'ENV'           0.0           1.0
RN1_CC  !num    name   comp number
        1      XE     2
        2      CS     1
        3      BA     2
        4      I2     2
        5      TE     2
        6      RU     2
        7      MO     2
        8      CE     2
        9      LA     2
        10      UO2    2
        11      CD     2
        12      AG     2
        13      BO2    2
        14      NA     3   ! Default H2O was replaced with Na for Na Chemistry
        15      CON    2
```

```
        16      CSI    2
        17      CSM    2
        18      H2OA   3   ! Added for Na Chemistry models
        19      NAOH   3   ! Added for Na Chemistry models
        20      NA2O2  3   ! Added for Na Chemistry models
        21      NA2O   3   ! Added for Na Chemistry models
  22  NAI    2   ! Added for NaI transport
!
! all new classes are required to input C7120, C7170
!   7130, 7136, 7141, 7102,  7111, 7120, 7131, 7132, 7170
!   7101, 7110
RN1_CSC 31 ! N  SCnumber   ClassName   Value       Index1     Index2
! vapor pressure
!!!             1  7110       H2OA         0.0     1          1
!!!             2  7110       H2OA        -1.0     1          2
!!!             3  7110       H2OA        10000.0  2          1
!!!             4  7110       H2OA        -1.0     2          2
!!!             5  7110       H2OA        -1.0     3          1
! vapor pressure
                1  7110   H2OA    3000.0    1         1
                2  7110   H2OA   18000.0    1         2
                3  7110   H2OA       8.875  1         3
                4  7110   H2OA       0.0    1         4
                5  7110   H2OA      -1.0    2         1
! molecular weight
            6  7120       H2OA        18.016      1
            7  7120       H2OA        18.016      2
! vapor pressure - set to same as UO2, except boiling point
            8  7110       NAOH        1663.0      1          1
            9  7110       NAOH        32110.0     1          2
            10  7110       NAOH        11.873      1          3
            11  7110       NAOH        0.0         1          4
! molecular weight
            12  7120       NAOH        39.99      1
            13  7120       NAOH        39.99      2
! vapor pressure - set to same as UO2 // changed boiling point from 1500.0 to 930.0 per https://en.wikipedia.org/wiki/Sodium_pero
            14  7110       NA2O2       930.0       1          1
            15  7110       NA2O2       32110.0     1          2
            16  7110       NA2O2       11.873      1          3
            17  7110       NA2O2       0.0         1          4
! molecular weight (wrong weight was shown here -- 78.98 --> 77.98)
            18  7120       NA2O2       77.98      1
            19  7120       NA2O2       77.98      2
! vapor pressure - set to same as UO2 // this guy sublimates at 1275 C and boils at 1950 C
            20  7110       NA2O        1275.0      1          1
            21  7110       NA2O        32110.0     1          2
            22  7110       NA2O        11.873      1          3
            23  7110       NA2O        0.0         1          4
! molecular weight
            24  7120       NA2O        61.98      1
            25  7120       NA2O        61.98      2
! vapor pressure
            26  7110       NAI        931.4     1          1
            27  7110       NAI        11895.0     1          2
            28  7110       NAI        12.525      1          3
            29  7110       NAI        2.5         1          4
! molecular weight
            30  7120       NAI        149.89      1
            31  7120       NAI        149.89      2


!! ! log10 [Pressure (mm Hg)] = -A / T + B + C log10 (T)
!!
!! ! https://pubs.aip.org/aip/jcp/article/16/11/1035/199477/The-Vapor-Pressures-of-Some-Alkali-Halides
!! ! logPmm= C-A (1000/T) +(2.5)*log(1000/T).
!! !
!! ! NaI
!! !
```

```
!! ! A
!! ! 11.895
!! !
!! ! Standard
!! ! deviation
!! ! of A
!! ! 0.14
!! !
!! ! c
!! ! 12.525
!! ! https://webbook.nist.gov/cgi/cbook.cgi?ID=C7681825&Mask=1E9F&Type=ANTOINE&Plot=on#ANTOINE
!! ! NIST has a source that is 1 year older and pretty much shows a vapor pressure of 0 at any
!! ! temperatures below 1100 K
!! ! note, AB7 experiment details NaI was heated up to 1151 K
!! ! N2 gas was mixed with this and it was noted that the N2 gas entered CSTF at 483 K
!! ! thus, its expected that NaI would not have been able to remain in vapor phase for any period of time
!
! *** AEROSOL SOURCES
! *
RN1_AS  'AS002' 'CSTF_lower' VAPOR 'NAI'  0.0 1.97E-4   TF 'ASOURCE2'
RN1_AS01      LOGNORMAL       5.44E-7          1.55
!)

RN2_INPUT
!)
!
! //// add NAC models
!            iactv
NAC_INPUT    0      !(
!            NaCL1    NaCL2      NaCL3    NaCL4       NaCL5
NAC_RNCLASS  H2OA     NA         NAOH     NA2O2       NA2O
!
            !n  CVHNAME   FNA2O
NAC_ATMCH 1
            1  'CSTF_upper'   0.0

!!!        !n   CVHNAME         FO2 FHEAT  FNA2O  FNA2O2 TOFF     DAB
NAC_PFIRE 1
   1  'CSTF_upper'    1.0    1.0    0.0    0.0    600.0    0.0
NAC_SPRAY 1
            !n  CVHNAME    HITE  DME      FNA2O2       SPRDT   SOU-TYPE  MASS-NAME   THERM-NAME   DROPVEL-NAME
            1  'CSTF_upper'   10.0  0.00318    1.0     -1.0       TF        'SPRAY-M'   'SPRAY-T'   'SPRAY-V'


end program melgen



program melcor

CVH_INPUT
CVH_ALLOWCOLDATM
CVH_SUPERCOOLPOOL
!block: 'melcorbase'

EXEC_INPUT !(
EXEC_TITLE 'Sensitivity test AB7'
EXEC_CPULEFT 10.0
EXEC_CPULIM 2500.0
EXEC_CYMESF 10 10
EXEC_EXACTTIME    1 !n          time
                    1         100.0
EXEC_JOBID 'REF'
EXEC_TIME    4 !n    time dtmax  dtmin   dedit dtplot  dtrest dcrest
                1     0.0   0.5 1.0E-3 10000.0   0.1 50000.0 1.0E10
                2    20.0   0.5 1.0E-3 10000.0   0.1 50000.0 1.0E10
                3  1000.0 100.0   0.01 10000.0   50.0 50000.0 1.0E10
                4 10000.0 100.0   0.01 10000.0  100.0 50000.0 1.0E10
```

```
EXEC_TEND 1.62E5
!)

end program melcor
```

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