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Benchmarking MELCOR's NAC Package to ABCOVE Tests AB5 and AB6

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ABSTRACT

This report presents analyses of the AB5 and AB6 ABCOVE sodium spray fire experiments 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. By analyzing the AB5 and AB6 experiments with and without the NAC package, sodium specificity for spray combustion and aerosol formation as well as speciation of the combustion products are reviewed with the new packages. This effort provides code users with a demonstration of the current code capabilities. This report provides the current best practices for the NAC package as well as a discussion of any issues observed while performing the presented analyses.

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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-Condensable 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 fast breeder reactors (LMFBRs) 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 behavior of molten sodium in the event of 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 and SPHINCS. 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 [7, 8]. 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).

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 user's may

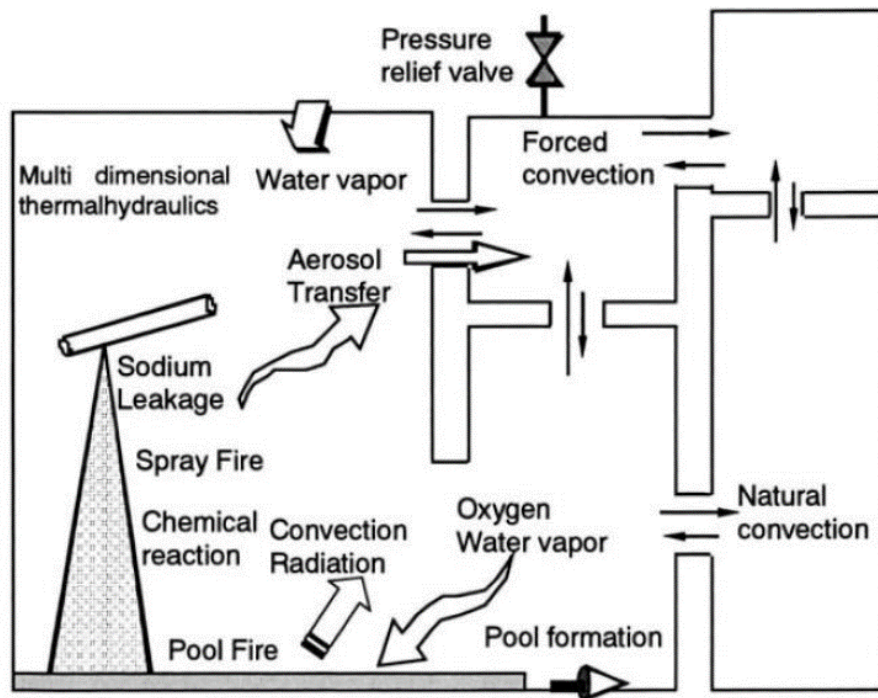


Figure 1-1 Models used in the SPHINCS and CONTAIN-LMR computer codes [9]. The partitions represent the separation of cells that can be used to model the transport of fluids between cells.

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 safe design and development of advanced reactors that incorporate molten Na into their build. This report will review the aerosol experiments, AB5 and AB6, and perform an analysis on the modeled sodium spray and fire behavior using MELCOR's NAC package. The AB5 and AB6 tests 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. AB5

Test AB5 was performed in September 1982 at HEDL. It involved the generation of a single-species aerosol by spraying molten Na into an air atmosphere [4]. The goal of this test was to validate aerosol behavior codes under the conditions that are analogous to a severe accident involving a high sodium leak rate in a sodium fast reactor. The test setup for AB5 of the ABCOVE program is shown in Figure 1-2 below.

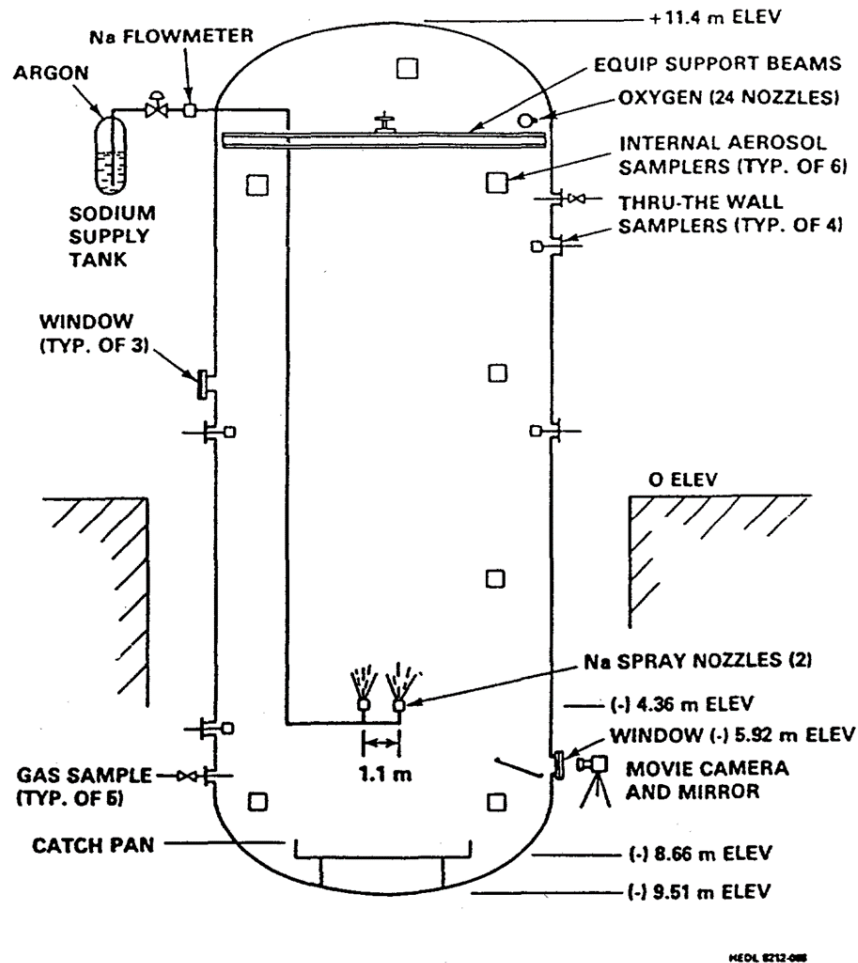


Figure 1-2 Setup of the CSTF containment vessel for AB5 [3].

For this test, 223 kg of commercial-grade, molten sodium was injected from an external supply tank into the CSTF containment vessel through two spray nozzles that were elevated 5.15m from the base of the vessel for a period of 872s. During the spray period, aerosol formation through Na combustion was observed and quantified. Analysis from the end of the experiment concluded the conversion of sodium through combustion resulted in the generation of aerosol as 60% Na_2O_2 and 40% NaOH . Note, the containment vessel was kept sealed for 5.136E5s or 5.94 days before any aerosol mass analysis was performed. A summary of the experimental conditions can be found in Table 1-2.

Table 1-2 Summary of Test AB5 conditions [3].

TEST CONDITION	VALUE
Initial Containment Atmosphere	
Oxygen Concentration	23.3±0.2%
Temperature (mean)	302.25K
Pressure	0.122MPa
Dew Point	289.15±2K
Nominal Leak Rate	1% per day at 68.9kPa
Na Spray	
Na Spray Rate	256±15g/s
Spray Start Time	13s
Spray Stop Time	885s
Total Na Sprayed	223±11kg
Na Temperature	836.15K
Spray Drop Size, MMD	1030±50µm
Spray Size Geom. Std. Dev., GSD	1.4
Oxygen Concentration	
Initial O ₂ Concentration	23.3±0.2 vol %
Final O ₂ Concentration	19.4±0.2 vol %
Oxygen Injection Start	60s
Oxygen Injection Stop	840s
Total O ₂	47.6m ³ (STD)
Containment Conditions During Test	
Maximum Average Atmosphere Temperature	552.15K
Maximum Average Steel Vessel Temperature	366.65K
Maximum Pressure	213.9kPa
Final Dew Point	271.65K
Aerosol Generation	
Generation Rate	445g/s
Mass Ratio, Total to Na	1.74
Material Density	2.50g/cm ³
Initial Suspended Concentration	0
Source Mass Median Radius	0.25µm
Source Sigma, σ_g	1.5
Maximum Suspended Mass Concentration	170g/m ³
Suspended Conc. Steady-State Value	110±17g/m ³

This test served to provide experimental data for the cases of a single-component aerosol source that was generated by a sodium spray in an air atmosphere. It also generated a wide-array of experimental data including the temperature and pressure of the containment vessel (see Table 1-1 for CSTF characteristics) as well as general characterization of the suspended and deposited aerosol during and after the implementation sodium spray source. Table 1-2 below details the test conditions for the AB5 experiment which include all the necessary parameters to model a sodium spray source into an initial containment atmosphere. 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.

1.2. AB6

Test AB6 was performed in July 1983 at HEDL. It involved the simultaneous release of aerosolized NaI in the presence of a sodium spray fire, which releases its own combustion aerosols [4]. The test setup for AB6 of the ABCOVE program is shown in Figure 1-3 below.

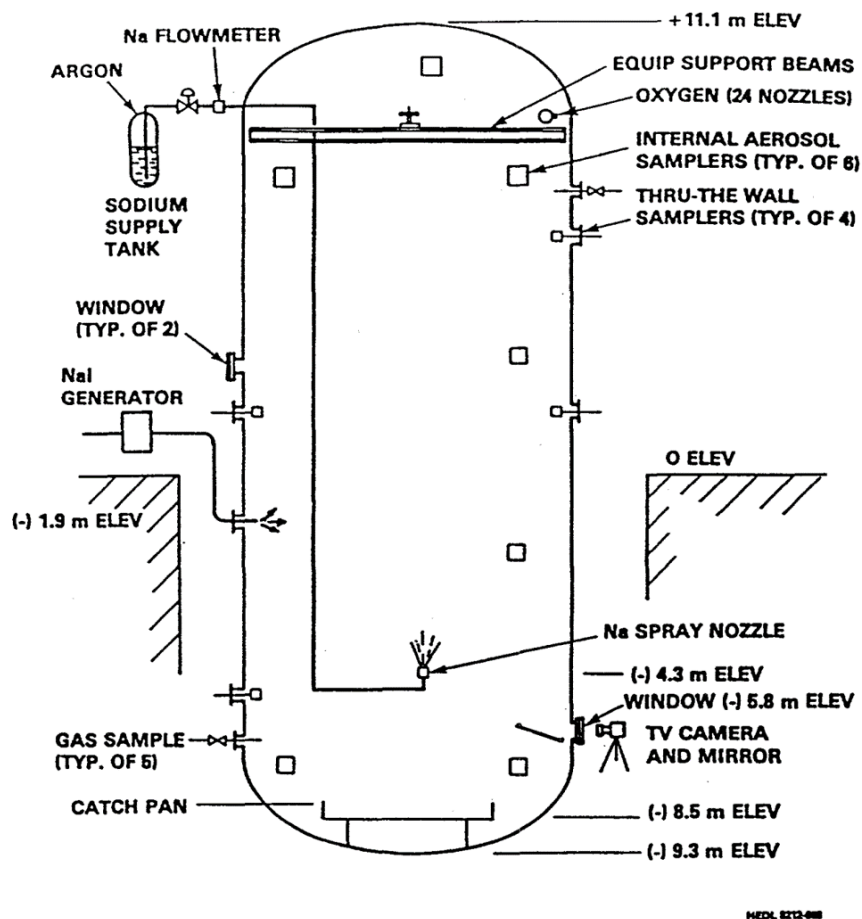


Figure 1-3 Setup of the CSTF containment vessel for AB6 [3].

A NaI aerosol was injected into the CSTF at the start of the experiment for a duration of 3000s yielding 420g of injected NaI. About 620s after the start of the injection of NaI, 204 kg of commercial grade, molten sodium was injected from an external supply tank into the CSTF containment through a single spray nozzle that was elevated at 5.0m from the base of the vessel for a period of 4780s. Like test AB5, this experiment yielded the sodium combustion aerosols: Na_2O_2 and NaOH . The containment vessel in this test was kept sealed for 2.77E5s or 3.206 days before any aerosol masses were analyzed. A summary of the experimental conditions can be found in Table 1-3.

For this test, NaI aerosol was released simultaneously with a sodium spray source where the primary goal was to show the coagglomeration behavior of two aerosol species and validate codes. Like AB5, this test generated thermal-hydraulic experimental data including the

Table 1-3 Summary of Test AB6 conditions [3].

TEST CONDITION	VALUE
Initial Containment Atmosphere	
Oxygen Concentration	23.9±0.2%
Temperature (mean)	304.15K
Pressure	114.2kPa
Dew Point	285.35K
Sodium Spray	
Sodium Spray Rate	42.8±2.1g/s
Spray Start Time	620s
Spray Stop Time	5400s
Total Na Sprayed	204.7±4.1kg
Sodium Temperature	833.15K
Spray Drop Size, MMD	640±40µm
Spray Size Geom. Std. Dev., GSD	1.4
Containment Conditions During Test	
Maximum Average Atmosphere Temperature	438.25K
Maximum Average Steel Vessel Temperature	352.05K
Maximum Pressure	169.5kPa
Final Dew Point	268.95K
NaOx Aerosol Source	
Start Time	620s
Stop Time	5400s
Release Rate	77.9±4g/s
Total NaOx Released	372.4±10kg
Material Density	2.45g/cm ³
Source 50% Radius	0.25µm
Source Sigma	2.0
Mass Ratio, Total to Na	1.82
NaI Aerosol Source	
Start Time	0s
Stop Time	3000s
Release Rate	0.14g/s
Total NaI Released	420g
Material Density	3.67g/cm ³
Source 50% Radius	0.272µm
Source Sigma	1.55

temperature and pressure of the containment vessel as well as the generation and behavior suspended and deposited aerosols. Table 1-3 details most of the test conditions for test AB6. This table, however, was found to be missing important information surrounding the injection of oxygen into the system as well as injection temperature of nitrogen gas coupled to the NaI source. Oxygen was injected into the CSTF at a rate of 0.021 kilograms per second from 60s to 4400s. Nitrogen gas was injected simultaneously with the NaI where its temperature was reported to be 483 K and the injection rate was 0.018 kilograms per second [1].

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 [10]. 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.

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 hypothetical 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 noncondensable 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 fire modeling within MELCOR, both modern and prior modeling methodologies, the simulation results of the AB5 and AB6 ABCOVE experiments utilizing a progressive modeling approach to demonstrate the importance of the various modeling options, and a demonstration of the sensitivities across select aerosol, sodium fire and atmospheric chemistry parameters to highlight the need for adequate characterization of aerosol agglomeration/behavior.

2.1. Modeling Sodium Spray Fire Accidents in MELCOR

There are two general approaches available to modeling sodium spray fires: 1) specifying the mass and energies related to the sodium spray fire as source terms to the code or 2) applying the NAC package and sodium EOS to directly compute the sodium spray fire behavior. The first modeling method is presented to elucidate the acceptability of historic sodium modeling analyses

as well as to provide a meaningful starting point for discussing the modeling progression leading to the use of the NAC package and sodium EOS. As many model developers are unfamiliar with using the NAC package, a more detailed discussion on the modeling methodology is given.

2.1.1. *Method 1: Sourcing in Reaction Heat and Aerosol Byproducts*

2.1.1.1. CVH_INPUT

CV_SOU	2 !n	ctyp	interp	iessrc	idmat
1	mass	rate	tf	'O2SOURCE'	O2
2	te	rate	tf	'O2TEMP'	-1

To achieve the appropriate thermal-hydraulic response, method 1 relies on quantifying the amount of heat generated from the reaction of the Na spray with the surrounding atmosphere using the experimental characterization of the aerosol deposits. This heat is incorporated into the model using a tabular function (TF_INPUT) to specify the timing and quantity of heat input, and the control volume source (CV_SOU) field to introduce it into the designated environment. Furthermore, the pressure increase in the containment resulting from input gas sources must be also considered. In the case of ABCOVE tests AB5 and AB6, oxygen and nitrogen are both introduced as gases into the system, utilizing the same method employed for inputting heat (i.e., tabular functions tied to the CV_SOU field).

2.1.1.2. TF_INPUT The TF_INPUT as follows:

```
!
!      tfname      tfscal      tfadcn
TF_ID      'O2SOURCE'      1.0      0.0 ! (
!      size
TF_TAB      6 !n
!      x      y
1      0.0      0.0
2      59.9      0.0
3      60.0      0.08718
4      840.0      0.08718
5      840.1      0.0
6      10000.0      0.0

!
!      tfname      tfscal      tfadcn
TF_ID      'O2TEMP'      1.0      0.0 ! (
!      size
TF_TAB      5 !n
!      x      y
1      0.0      302.25
2      60.0      302.25
3      840.0      302.25
4      840.1      302.25
5      10000.0      302.25

!
!      tfname      tfscal      tfadcn
TF_ID      'EXHEAT'      1.0      0.0 ! (
!      size
TF_TAB      5 !n
!      x      y
1      0.0      0.0
2      12.9      0.0
3      13.0      3.31E5
4      885.0      2.89E9
5      5.136E5      3.05E9
```

```

!)
! TABULAR FUNCTION FOR AEROSOL SOURCE
!
!
!               tfname               tfscal               tfadcn
TF_ID           'ASOURCE'           1.0                 0.0 !
!
! size
TF_TAB          5 !n                x                    y
!
!               1                0.0                0.0
!               2               12.95               0.0
!               3               13.0                1.0
!               4              885.0                1.0
!               5              886.0                0.0
!
!)
```

2.1.1.3. RN1_INPUT Additionally, all produced aerosols are introduced using the RN packages fields RN1_AS and RN1_AS01, where tabular functions define the quantity and rate of aerosol introduction into the system. MELCOR utilizes the imported heat and gas sources to establish the correct thermal-hydraulic conditions and disperse the aerosol sources throughout the specified control volume homogeneously.

	name	ivol	iphs	iclss	rfrs	xm	itab	cfnam
RN1_AS	'AS000'	'CSTF'	VAPOR	'CS'	0.0	0.445	TF	'ASOURCE'
!		idist		geommm			gsd	
RN1_AS01		LOGNORMAL		5.0E-7			1.5	

It is important to note that this method does not directly account for the actual quantity of sodium released in a spray fire scenario, nor does it consider the orientation of the spray or the temperature of the molten sodium source. Instead, it uses the Cs class as a surrogate to model the transport behavior of a sodium oxide aerosol. Furthermore, test AB6 utilizes the CsI class to track sodium iodide. As a result, without direct knowledge of the generated aerosols, this method quickly becomes inadequate for predicting aerosol formation and releases from any given sodium accident since molten sodium reacting with an air atmosphere produces oxide byproducts that emit heat. The subsequent section on the NAC package aims to address this limitation by directly modeling the sodium chemistry involved in a sodium spray fire.

2.1.2. Method 2: Using the Sodium Chemistry (NAC) Package in MELCOR

The MELCOR NAC package incorporates sodium chemistry models to analyze potential liquid sodium incidents, such as coolant loss events leading to spray and/or pool fires. Sodium undergoes exothermic reactions with oxygen and water in the air, resulting in energy release and the formation of sodium oxide aerosols. These phenomena are crucial to model for Level 2 and 3 probabilistic analyses, as well as to accurately characterize the timing and scale of any environmental release in hypothetical accidents in advanced sodium-cooled reactor designs.

The sodium chemistry models integrated into MELCOR are based on the CONTAIN-LMR code, 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 consult the NAC users' guide.

2.1.2.1. NAC_INPUT Enabling the NAC_INPUT facilitates sodium spray-fire modeling within user-defined control volumes, encompassing the determination of sodium reacted, energy generation, and oxide mass production. The sodium spray model utilized in MELCOR is rooted in a JAEA-modified version of the NACOM code developed by Brookhaven National Laboratory [11].

The sodium spray model within the NAC package encompasses essential tools for effectively simulating a sodium spray accident. To utilize this package, users must first specify the control volume of interest (CVHNAME) and the height of the spray source within the problem (HITE). Additionally, the mass mean diameter of the spray droplets (DME) must be defined for combustion modeling and mass burn rate calculations. Users should also define the mole fraction of sodium peroxide produced from combustion (FNa_2O_2), establish a time step for the spray combustion (SPRDT), and specify the source type (SOU-TYPE) as either a tabular or control function. The last three parameters define the mass, temperature, and velocity of the sodium spray sources, also as tabular or control functions. Note, the last field, SPRAY-V, is optional and not required to be able to run the NAC_SPRAY field, however, if left out, SPRDT must be set equal to -1.00 instead of 0.00. An example of the input structure can be found below:

```
NAC_SPRAY 1
!n CVHNAME HITE DME FNA2O2 SPRDT SOU-TYPE MASS-NME THERM-NME DRPVEL-NME
1 'CSTF' 5.15 0.00103 1.0 0.00 TF 'SPRAY-M' 'SPRAY-T' 'SPRAY-V'
```

The atmospheric chemistry model encompasses the sodium interactions with atmospheric constituents not directly addressed by the sodium spray model. It calculates the reaction rates for sodium and sodium oxides in various states or locations across different MELCOR packages, involving phenomena such as film condensation, aerosol reactions, agglomeration, and transformations. A list of the atmospheric chemical reactions that are present within the NAC package can be found in the Table below. Given the exothermic nature of these reactions, enabling this package is expected to introduce a thermal load to the containment system. While the atmospheric chemistry model within the NAC package is implemented in the code, it is not explicitly documented in the user's guide [10] as an enabled parameter. Enabling this model

requires specifying record, NAC_ATMCH, the control volume of interest (CVHNAME), such as "CSTF," and a mole fraction of Na₂O (FNA2O), a floating-point number between 0.0 and 1.0. An example of the input structure can be found below:

```
NAC_ATMCH 1
!n CVHNAME FNA2O
1 'CSTF' 0.0
```

The presence of water is still necessary in the system even when the atmospheric chemistry model is activated, as enabling NAC makes the default fluid in the system sodium, not water. Thus, water must be sourced in through another means.

Table 2-1 Atmospheric Chemistry Reactions Data and Applications [10].

#	Reaction	Reaction Heat	Locations
1	$\text{Na} + \text{H}_2\text{O} (\text{l}) \rightarrow \text{NaOH} + \frac{1}{2} \text{H}_2$	$\Delta H_{\text{NaOH}} - \Delta H_{\text{H}_2\text{O}}$	Reactions within aerosol particles or within aerosol deposit or condensable film
2	$2 \text{Na} + \text{H}_2\text{O} (\text{g}) \rightarrow \text{Na}_2\text{O} + \text{H}_2$	$\Delta H_{\text{Na}_2\text{O}} - \Delta H_{\text{H}_2\text{O}}$	Reactions with gases, aerosols with gases, and deposits or film with gases
3	$2 \text{Na} + (1 - 0.5 \cdot f_{\text{ox}}) \text{O}_2 \rightarrow f_{\text{ox}} \cdot \text{Na}_2\text{O} + (1 - 0.5 \cdot f_{\text{ox}}) \cdot \text{Na}_2\text{O}_2$	$f_{\text{ox}} \cdot \Delta H_{\text{Na}_2\text{O}} + (1 - f_{\text{ox}}) \cdot \Delta H_{\text{Na}_2\text{O}_2}$	Reactions of gases with gases, aerosols, and deposits/film
4	$\text{Na}_2\text{O}_2 + 2 \text{Na} \rightarrow 2 \text{Na}_2\text{O}$	$\Delta H_{\text{Na}_2\text{O}} - 0.5 \Delta H_{\text{Na}_2\text{O}_2}$	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	$\text{Na}_2\text{O} + \text{H}_2\text{O} (\text{g}) \rightarrow 2 \text{NaOH}$	$\Delta H_{\text{NaOH}} - 0.5 (\Delta H_{\text{Na}_2\text{O}} + \Delta H_{\text{H}_2\text{O}})$	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	$\text{Na}_2\text{O}_2 + \text{H}_2\text{O} (\text{g}) \rightarrow 2 \text{NaOH} + \frac{1}{2} \text{O}_2$	$\Delta H_{\text{NaOH}} - 0.5 (\Delta H_{\text{Na}_2\text{O}_2} + \Delta H_{\text{H}_2\text{O}})$	

As the NAC package currently exists, only reactions 3 and 6 are functional in the code. This creates a limitation on the actual behavior of the aerosol speciation during the AB5 and AB6 tests. Ideally, having competing reactions in the system would serve to better model reality and provide more accurate predictions.

2.1.2.2. NCG_INPUT Water must be included in the atmosphere of the control volume "CSTF" as a non-condensable gas through the parameter "H2OV," as detailed in the reference

manual's NAC section. Additionally, the NAC model requires 'H2' to be present as a non-condensable gas (set its mass fraction to 0.0 if also not initially present in your atmosphere), as it is a product from reaction 1 in the atmospheric chemistry model. Note, an error will be thrown if 'H2' is left out of the composition of your non-condensable gases. Thus, under the NCG_INPUT, the following must be present:

```

NCG_ID      'N2'
NCG_ID      'O2'
NCG_ID      'H2OV'
NCG_ID      'H2'

```

2.1.2.3. CVH_INPUT While under the CVH_INPUT, these gases are plugged in with their relative mass fractions:

```

!
CV_NCG      nmmat      ncgid      tdew
!            4          RHUM      0.0
!            n          namgas      mass
!            1          'N2'       0.7558
!            2          'O2'       0.2296
!            3          'H2OV'     0.0146
!            4          'H2'       0.0000

```

To add gas *sources* such as O₂, to a desired containment vessel or region, the following must be input to CVH_INPUT as a control volume source:

```

CV_SOU      2 !n      ctyp      interp      iessrc      idmat
1 mass      rate      tf        'O2SOURCE'    O2          1.0
2 te        rate      tf        'O2TEMP'     -1

```

2.1.2.4. TF_INPUT Where the referenced tabular functions ('tf') 'O2SOURCE' and 'O2TEMP' must exist in the TF_INPUT as follows:

```

!
TF_ID      tfname      tfscal      tfadcn
!           'O2SOURCE'  1.0          0.0 ! (
! size
TF_TAB      6 !n      x          y
!           1          0.0         0.0
!           2          59.9        0.0
!           3          60.0        0.08718
!           4          840.0        0.08718
!           5          840.1        0.0
!           6          10000.0      0.0
!
!
TF_ID      tfname      tfscal      tfadcn
!           'O2TEMP'    1.0          0.0 ! (
! size
TF_TAB      5 !n      x          y
!           1          0.0         302.25
!           2          60.0        302.25
!           3          840.0        302.25
!           4          840.1        302.25
!           5          10000.0      302.25

```

For the NAC_INPUT, the NAC_SPRAY field requires the following tabular functions within the TF_INPUT to satisfy the optional fields specified previously as the spray mass, velocity and temperature.

```

!
!      tfname      tfscal      tfadcn
TF_ID      'SPRAY-M'      1.0      0.0 ! (
!      size
TF_TAB      6 !n      x      y
      1      0.0      0.000
      2      12.9      0.000
      3      13.0      0.256
      4      885.0      0.256
      5      885.1      0.000
      6      10000.0      0.000

!
!      tfname      tfscal      tfadcn
TF_ID      'SPRAY-T'      1.0      0.0 ! (
!      size
TF_TAB      6 !n      x      y
      1      0.0      0.000
      2      12.9      0.000
      3      13.0      836.15
      4      885.0      836.15
      5      885.1      0.000
      6      10000.0      0.000

!
!      tfname      tfscal      tfadcn
TF_ID      'SPRAY-V'      1.0      0.0 ! (
!      size
TF_TAB      6 !n      x      y
      1      0.0      0.000
      2      12.9      0.000
      3      13.0      -5.216
      4      885.0      -5.216
      5      885.1      0.000
      6      10000.0      0.000

!
!      iactv
NAC_INPUT      0      ! (
!      NaCL1      NaCL2      NaCL3      NaCL4      NaCL5
NAC_RNCLASS      H2OA      NA      NAOH      NA2O2      NA2O

```

2.1.2.5. RN1_INPUT The RN1_INPUT must change the 'numcls' field from 17 to 21 to accommodate the additionally defined/required RN classes for the NAC package (this accomodates: H2OA, NAOH, NA2O2, NA2O; if more or less classes are needed, increase or decrease the 21 to what fits):

```

!
!      numsec      numcmp      numcls      numca
RN1_DIM      20      3      21      6

!
!      !num      name      comp      number
RN1_CC      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
!
RN1_CSC 25 ! N  SCnumber  ClassName  Value      Index1  Index2
! 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
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
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
18 7120      NA2O2     77.98     1
19 7120      NA2O2     77.98     2
! vapor pressure
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

```

The classes must also be updated in the RN1_CC field as shown above where for each newly defined class, the vapor pressure and molecular weight must be defined under RN1_CSC. Note, class 14 replaced H2O with NA.

2.1.2.6. DCH_INPUT The updated RN classes must be reflected in the DCH classes as shown below:

```

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 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'

```


3. RESULTS & DISCUSSION

The direct-sourcing model, method 1, was built in MELCOR 1.8.2, converted to MELCOR 1.8.6 using SNAP [12], 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, method 2, was built and executed using MELCOR 2.2 (r2024.0.0) to provide a direct code-to-code comparison of the traditional MELCOR methodology (method 1) to today's implementation of the NAC package (method 2). Several plots and tables from Souto [3] are presented and refreshed with the added data generated from implementing method 2. 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 model utilizing method 2. In addition, experimental results show that the overall production of Na_2O is negligible and/or had been converted to NaOH , therefore, it was not modeled or accounted for and was assumed to be zero for both AB5 and AB6 models.

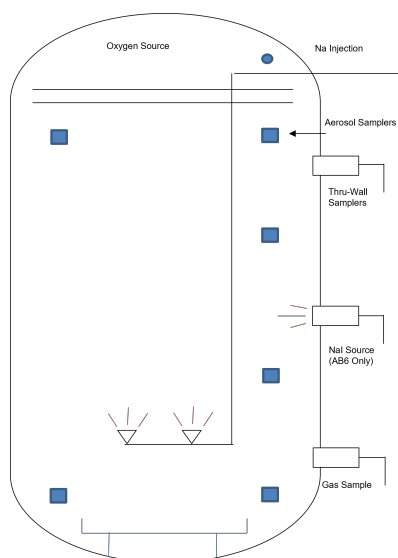


Figure 3-1 CSTF Containment Vessel.

The material of the heat structures was updated in the model employing method 2. The miscellaneous parameters for aerosols were kept consistent with Souto's analysis to maintain equivalent aerosol physics for a more direct comparison to that study.

!	chi	gamma	fslip	stick
RN1_MS00	1.5	2.25	1.37	1.0
!	turbds	tkgop	ftherm	deldif
RN1_MS01	1.0E-3	0.05	1.00	1.0E-5

In addition, a sensitivity study involving perturbations about the default parameters was performed on DME, SPRAY_V, FNA2O2, H2OV, RHONOM, CHI, GAMMA and STICK. The results for AB5 and AB6 can be found in Appendices A and B, respectively.

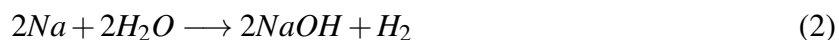
3.1. AB5

3.1.1. Summary

The NAC package was utilized to evaluate the anticipated aerosol and energy generation characteristics of the AB5 test. The results were compared against a previous MELCOR assessment utilizing method 1 and experimental results. A comparison of the plating and deposition values with the AB5 test data and previous MELCOR analyses using method 1 is outlined in Table 3-1. Method 2's energy generation and dissipation revealed potential issues tied to an exaggerated thermal-hydraulic response coupled with less energy generated than was input for method 1, which provided a more palatable set of responses. 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 response issues as sources dictate approximately 35% of the generated heat of a fire goes directly to the surrounding heat structures [13]. The deposition behavior of the aerosol species using method 2 was found lacking, while the suspension behavior was agreeable, when compared with experimental data and method 1.

3.1.2. Aerosol Behavior

3.1.2.1. Production Mechanisms for NaO_x Aerosols The production mechanisms of Na-based aerosols can be found in Table 2-1. For the chemical reactions involving the *direct* production of Na₂O₂ and NaOH from Na:



The maximum amount of Na₂O₂ and NaOH that could be generated, assuming all 223 kg injected Na solely underwent either respective reaction, was determined to be 378 kg and 388 kg, respectively. Experimental results, shown in Table 3-1, report 402.80 kg NaO_x deposited.

It is suspected that mass was added to the final mass determined for aerosol deposition as indicated in the report for test AB5 [2] where they determined a 10% excess in sodium content over the presumed injection amount of 223 kg. [2] concluded that the measurement of the 223 kg Na injection was accurate to within 1-2% and the data from deposition measurement was deemed less reliable. Given the total deposition of test AB5 was determined to be 402.8 kg with a 10% error (biased as 10% too high), the actual value is expected to be roughly 360 kg. The results using method 2 only yield 333.10 kg for deposited aerosols revealing a gap in the production mechanisms involved in modeling this experiment. One possible attribution to this error is the amount of water in the CSTF was not well characterized (see Section A.1.1). Another issue highlighted is the reasoning given for the spray drop size in section 4.2.3 of [2], which corresponds to the DME value in the NAC_SPRAY input. There is not a well-established connection between the spray size distribution of water droplets to sodium droplets other than a pressure drop across the nozzle. No characteristics are given about the temperature of the sodium

Table 3-1 ABCOVE test AB5 deposition results comparison between MELCOR using method 1 [7], MELCOR using method 2 (NAC-enabled) and test AB5 experimental data.

STRUCTURE	MELCOR	MELCOR-NAC				TEST AB5	
Plated Mass	NaOx (kg)	NaOH (kg)	+	Na2O2 (kg)	=	NaOx (kg)	NaOx (kg)
Top Head	1.60	0.23	+	0.81	=	1.04	0.96
Cylindrical Walls	18.10	2.96	+	11.68	=	14.61	17.75
Internal Components (Vertical)	3.82	1.20	+	2.68	=	3.88	N/A
Total Plated*	23.52	4.39	+	15.13	=	19.53	18.70
Settled Mass	NaOx (kg)	NaOH (kg)	+	Na2O2 (kg)	=	NaOx (kg)	NaOx (kg)
Bottom Head	190.00	22.56	+	138.65	=	161.21	200.10
Internal Components (Horizontal)	176.50	21.34	+	131.02	=	152.36	184.00
Total Settled^	366.50	43.91	+	269.37	=	313.57	384.10
Total Deposited	390.02	48.30	+	284.80	=	333.10	402.80

Experimental Error: *30%, ^10%

(density changes) or the surface tension differences between both fluids compared. A sensitivity study on the DME was performed to showcase its effects on the poor characterization of DME (see Section A.2.1). The value of DME is directly tied to the amount of sodium that combusts in the atmosphere, given the fall height and spray velocity values are fixed. From the NAC package, the NAC-SPR-NABM and NAC-SPR-NAPM plot records detail the burned mass and pooled mass of sodium, respectively. The amount of sodium burned in the NAC-enabled model was found to be only 196 kg out of the 223 kg injected in the system. The sensitivity study for DME shows that it does not require a substantial change toward a smaller size for most, if not all of the sodium to combust. The NAC package is able to output the change in masses of reactants and products for each equation (see Table 2-1) involved in atmospheric chemistry modeling. Using this information, it was found that reaction 1 of Table 2-1 is not enabled or active while using water defined as a noncondensable gas. It is suspected that if water vapor were modeled under the RN class that this reaction may proceed, however, it has not been tested. Therefore, the production mechanism of NaOH is solely dependent on the Na₂O₂ content in the atmosphere at a given time to support the reactants of reaction 6 in Table 2-1.

3.1.2.2. Deposition of Aerosols onto Heat Structures The results depicting the deposition of aerosol species onto the heat structures ('top-head', 'cylindrical walls', 'internal components (vertical)', 'bottom-head', and 'internal components (horizontal)') are presented in Table 3-1 above. The findings regarding the plated aerosol species of NaOx (where NaOx represents the cumulative mass of all sodium oxide species) were consistent with previous MELCOR results while the settled mass was underpredicted. Method 2 demonstrated notably improved prediction of the plated mass compared to method 1, taking into account that experimental results likely summed the cylindrical walls and internal components (vertical) measurements as one. The total deposited mass within the containment for method 2 was about 30 kg short from experimental observations, after taking into account the ≈10% excess mass.

However, certain differences were noted, particularly in the settled masses. Given that the model implementing method 2 uses Na as its working fluid, a percentage of the Na may not combust, leading to a portion of the masses being directed to a separate 'pool' mass region. It is important to note that any aerosols entering the height of the pool mass region, regardless of the minimal amount of pool mass present, will be transferred from a settled volume onto a heat structure. This mechanism was identified as a means of removing settled masses from the bottom head and internal components. In order to maintain consistency with previous work conducted by Souto [3], the results from using method 2 detail that the settled mass between the bottom head and internal components encompass a 50/50 split between aerosols settled in the 'pool' volume, as indicated by the plot parameter 'RN1-TYCLLIQ'. The experimental plated mass also exhibited differences when compared to the computationally determined masses, which may be attributed to the washing/sampling methods used for mass collection, as previously mentioned. For the same chemical reactions defined previously above, it is suspected that mass may have been added to the final mass determined for aerosol deposition, assuming the same wash methods were used for aerosol deposition as in test AB5.

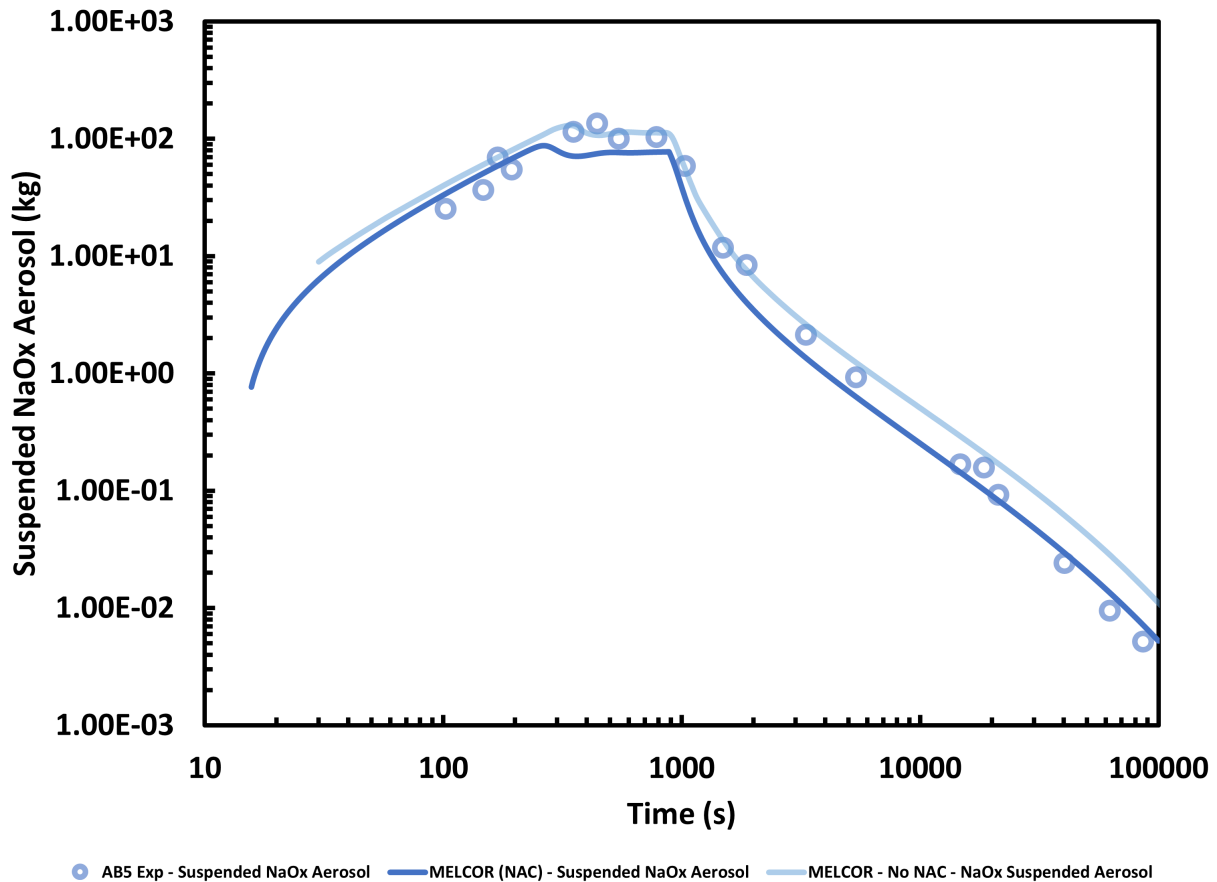


Figure 3-2 Suspended aerosol plots for the AB5 test.

3.1.2.3. Suspended Aerosols in Atmosphere The suspended aerosol behavior between methods 1 and 2 demonstrate a high level of agreement. This behavior was expected since the miscellaneous parameters for the aerosols were kept consistent with Souto's analysis. Sensitivity studies were also done on the GAMMA (see Section A.3.2) and CHI (Section A.3.3) parameters to showcase their strong effects for suspended aerosol species and how they influence deposition onto heat structures vs. into the pool mass.

3.1.3. Energy Generation & Dissipation

3.1.3.1. Thermal-hydraulic Response Figure 3-3 below compares the temperature and pressure plots between method 1, 2 and the experimental data.

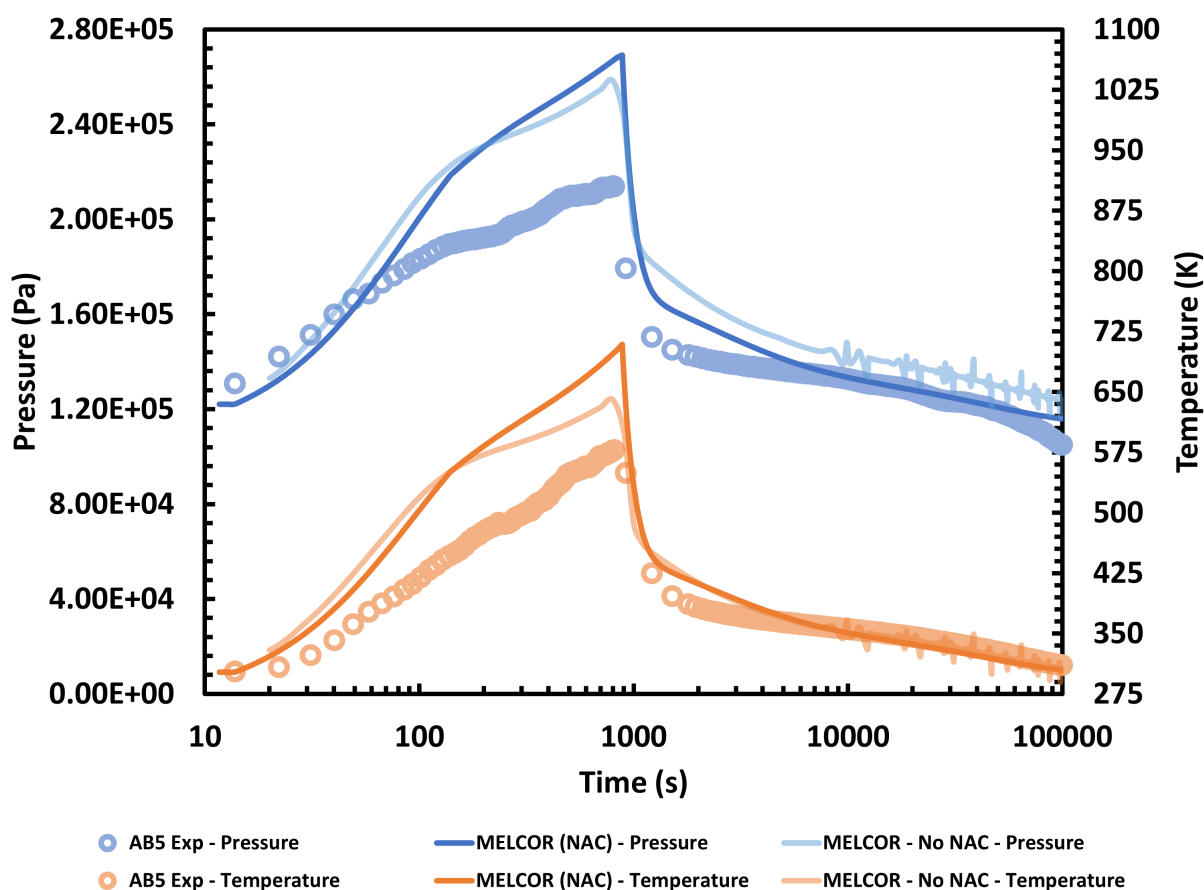


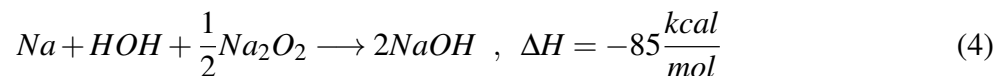
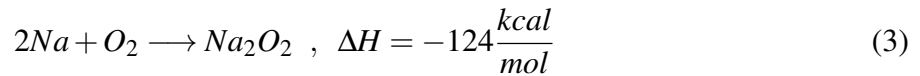
Figure 3-3 Pressure/Temperature plots for the AB5 test.

The results of AB5 employing method 2 gave slightly higher results pertaining to energy generation and energy dissipation than expected. The pressure and temperature response of this model appear to be harboring a large amount of heat input into the system which is causing excess temperature and pressure spikes in the system. This leads back to the statement within the summary regarding heat transfer from combustion to the walls. MELCOR is not specifically a

fire code and does not apply consideration for a flame's radiative heating effects to surrounding structures. Other programs, such as CFAST, apply a nominal radiative heat transfer fraction to the structures of 0.35 [13]. The removal of 35% of the energy dumped directly in to the atmosphere from combustion would create a much more gradual increase in pressure and temperature of the system as shown experimentally in Figure 3-3.

Given the large temperature increase of the models using method 2, the amount of heat introduced to the system using NAC would appear to be much greater than the heat explicitly input into the system through non-NAC enabled models (2.89 GJ; this number was determined in Souto's assessment using simple chemical reaction's heat of formation for two products; see Eq. 3 and 4). This was determined to not be the case when reviewing the energy added to the atmosphere through the NAC package's NAC-SPR-EA plot output. This particular lack of agreement leaves room for questions regarding how NAC generates, propagates and disperses heat in the CSTF vessel and atmosphere. Method 1, which uses the 2.89 GJ value, was found to still be overpredicting the experimental results but by less of a margin. Both models are presumed to be suffering from the same lack of radiative heat transfer to the surrounding structures as described previously MELCOR, with or without NAC enabled, does not perform this function. As a final note, Souto's model does not take into account input gases into the system, meaning it is underestimating the pressure of the CSTF. This discrepancy is presumed to be the cause for the slight difference between Souto's assessment and the present work.

3.1.3.2. Combustion Mechanisms To determine the amount of energy to add to the system, the models using the traditional methodology, as in method 1, rely on the calculation of the energy released during the following chemical reactions:



The total energy released from each these reactions, given as Q_1 and Q_2 , respectively, are as follows:

$$Q_1 = \left(\frac{0.6 \cdot (223 \times 10^3 g)}{2 \cdot (22.99 \frac{g}{mol})} \right) \cdot \left(124 \frac{kcal}{mol} \right) \cdot \left(4.184 \times 10^3 \frac{J}{kcal} \right) \quad (5)$$

$$Q_2 = \left(\frac{0.4 \cdot (223 \times 10^3 g)}{2 \cdot (22.99 \frac{g}{mol})} \right) \cdot \left(85 \frac{kcal}{mol} \right) \cdot \left(4.184 \times 10^3 \frac{J}{kcal} \right) \quad (6)$$

The resultant values yield a total energy released of 2.89 GJ for 223 kg Na injected into the system producing 60% Na_2O_2 and 40% NaOH. Note, it was determined experimentally that 60% of the mass fraction of the deposited aerosol was Na_2O_2 while the remaining 40% was NaOH. Additionally, a sensible energy gained to the system by energy imparted from the molten sodium was given as follows:

$$Q_s = (223 \times 10^3 g) \cdot (1.303 \frac{J}{g \cdot K}) \cdot (\Delta T) \quad (7)$$

where ΔT is the difference in temperature of the sodium to the containment (836.15 K - 302.25 K), 223×10^3 g is the mass of molten Na and $1.303 \frac{J}{gK}$ refers to the specific heat capacity of Na. The total added sensible energy imported was determined to be 0.155 GJ. As a result, 2.89 GJ of energy was directly input as a heat source in the non-NAC enabled models for the first 885 seconds while the last 0.155 GJ was added to the system gradually until the end of the model run-time (1×10^5 s).

3.1.3.2.1. Combustion in NAC When reviewing the energy added to the atmosphere from the NAC package in method 2, it became evident that there was a loss or discrepancy with respect to the energy transferred to the system. The energy input to the system using the NAC package was calculated to be 2.15 GJ. This energy could only have come from the sum of energies from reaction's 3 and 6 of Table 2-1. The deposited mass contained approximately 15% NaOH and 85% Na_2O_2 (see Table 3-1). Considering the dew point (289.15 ± 2 K) and mean temperature (302.25 K) of the atmosphere (see Table 1-2), the air's moisture content was determined to yield an H_2O mass fraction of 0.0146, based on calculations from the national oceanic and atmosphere administration (link). Given that this mass fraction corresponded to only 10 kg of H_2O was available in the atmosphere, the maximum NaOH production was estimated to be 44 kg using Eq 3, note, the NAC-based determination yielded 48.30 kg of NaOH (Table 3-1). Consequently, it is inferred that a higher humidity level in the system led to the increase in NaOH production from 15% to 40%.

The SPRAY-V variable controls how fast the spray droplets are moving upward (or downward) from their starting height, HITE (5.15 m). Thus, the faster the spray droplet is moving, the longer (or shorter) it has to fully combust through its arc in the atmosphere. This expectation is realized in the sensitivity plots found in Section A.2.3.

3.1.3.2.2. Calculation of SPRAY_V The spray velocity for a 3-8ba-15 hollow cone nozzle was calculated as follows:

$$v = \frac{m_{flow}}{\rho \times A \times n} \quad (8)$$

where v is the nozzle exit velocity ($m s^{-1}$), m_{flow} is the mass flow rate out of the nozzle ($kg s^{-1}$), ρ is the density of the fluid ($kg m^{-3}$), A is the cross-sectional area of the nozzle (m^2), and n is the # nozzles present. The mass flow rate is given by experimental measurements to be $0.256 kg s^{-1}$. The density of the molten sodium at $563^\circ C$ was determined to be $816.88 g cm^{-3}$ through interpolation of tabulated values for molten sodium density at $500^\circ C$ and $600^\circ C$. The nozzle cross sectional area was calculated to be $2.43E-05 m^2$ by using the vendor's given nozzle diameter, $5.56E-3$ m. The # nozzles used in the experiment was 2. The resultant velocity coming out of each nozzle was determined to be $6.45 m s^{-1}$. This velocity is with respect to an exit angle of 52° in a hollow cone emission separated by 72° . Thus, the z-directional velocity must be calculated to be imported into MELCOR's NAC model which only has the ability to dictate an upward or downward direction. The velocity in the z-direction was determined to be $5.22 m s^{-1}$. Note, the velocity must be input as a negative value to dictate +z direction (upward).

3.2. AB6

3.2.1. Summary

The NAC package was utilized to evaluate the anticipated aerosol and energy generation characteristics of the AB6 test. The results were compared against a previous MELCOR assessment utilizing method 1 and experimental results. The aerosol plating and deposition behavior in test AB6 was examined in MELCOR using method's 1 and 2. The results were then tabulated to compare against experimental data. A comparison of these values is shown in Table 3-2 below. The energy generation and dissipation of the model implementing method 2 was observed through the thermal-hydraulic responses given in the pressure and temperature plots and the total energy input in the system through chemical reactions occurring through the NAC package. Unlike test AB5, radiative heat transfer from the combustion flame to the walls was not an issue for the thermal-hydraulic response of the CSTF because of the more gradual insertion of Na spray into the system over a longer period of time.

3.2.2. Aerosol Behavior

3.2.2.1. Production Mechanisms for NaO_x Aerosols As in AB5, the production mechanisms of the Na spray aerosols within the NAC package can be found in Table 2-1. It was determined experimentally that the combustion aerosols generated for test AB6 were composed of either Na₂O₂ and NaOH. Thus, as in test AB5, it was assumed that only Na₂O₂ and NaOH were produced and that reactions 3 and 6 of Table 2-1 were the only reactions that were utilized in the NAC package.

3.2.2.2. Production Mechanism for NaI Aerosol NaI was sourced as a aerosol using the RN1_AS and RN1_AS01 records. A snippet of the code is found below and in Section C.2 in the Appendix.

```
RN1_AS 'AS002' 'CSTF' VAPOR 'NAI' 0.0 1.4E-4 TF 'ASOURCE2'  
RN1_AS01 LOGNORMAL 5.44E-7 1.55
```

A new class was also required and 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 nitrogen source was defined as a control volume source with a simultaneously release time as the NaI source. The nitrogen was the carrier gas for the NaI insertion.

3.2.2.3. 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 3-2 above. Overall, the results of the plated and settled aerosol species of NaI and NaO_x (where NaO_x is defined as the sum of all sodium oxide species) were consistent with the previous MELCOR results: the plated mass was heavily under-predicted while the settled mass was slightly over-predicted. Overall however, the total deposited mass in the containment for method 2 was found to be agreeable with the experiment.

Table 3-2 ABCOVE test AB6 deposition results comparison between MELCOR using method 1 [7], MELCOR using method 2 (NAC-enabled) and test AB6 experimental data.

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	0.03	+	0.25	=	0.21	0.21	1.58 1.68
Cylindrical Walls	11.00	13.00	1.14	+	8.31	=	10.89	10.89	35.80 46.51
Internal Components (Vertical)	1.28	2.85	0.37	+	0.91	=	2.82	2.82	N/A N/A
Total Plated*	12.68	16.23	1.55	+	9.47	=	11.02	13.92	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	14.75	+	156.62	=	171.37	206.31	156.07 195.60
Internal Components (Horizontal)	172.00	195.00	13.97	+	148.17	=	162.13	195.46	179.00 172.60
Total Settled^	358.00	404.00	28.72	+	304.79	=	333.51	401.77	335.07 368.20
Total Deposited	370.68	420.23	30.27	+	314.26	=	344.53	415.69	372.45 416.39

Experimental Error: *30 %, ^10%

There were several noted differences such as those found in the settled masses. Because method 2 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. 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 as mentioned earlier. For the same chemical reactions defined for test AB5, (Eq. 3, Eq. 4) the maximum amount of Na₂O₂ and NaOH that could be generated, assuming all 204 kg injected Na underwent each respective reaction, was determined to be 345 kg and 355 kg, respectively. 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 leading to an excess mass of up to 10%.

3.2.2.4. Suspended Aerosols in Atmosphere Two separate plots are shown in Figure 3-4 detailing the suspended aerosols of NaI and NaO_x. The plot parameter 'RN1-TYCLAIR' was called for method 2 to plot the airborne mass of a defined class (i.e. aerosol species) while existing data from Souto used the 'RN1-ATRG' to plot the total radioactive aerosol in the gas phase for method 1.

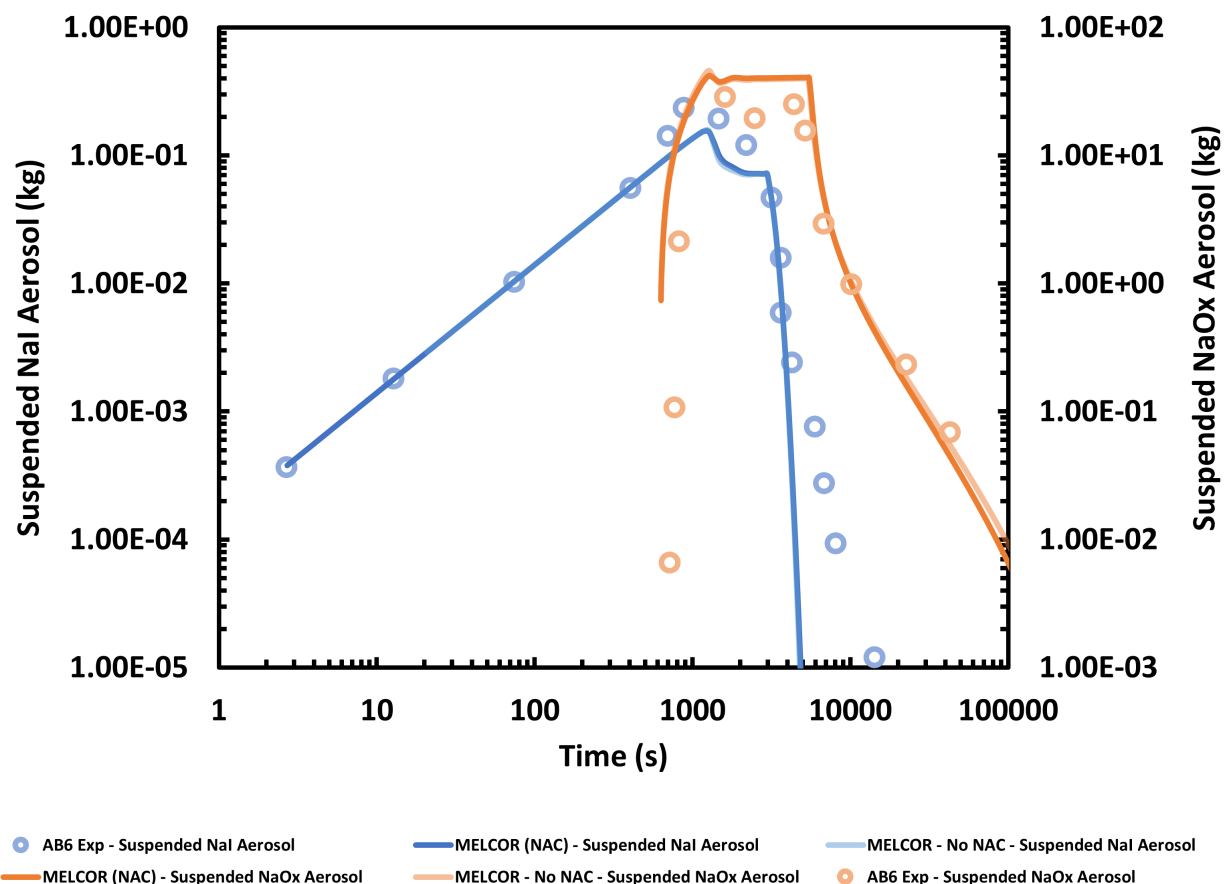


Figure 3-4 Suspended aerosol plots for the AB6 test.

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 NaO_x aerosol, whose density from test AB5 was reported out to be 2500 kg m⁻¹. 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. Sensitivity perturbations were applied to these key aerosol parameters (see Section B) and found to greatly control the suspended aerosol levels. Re-suspension of the NaI aerosol, seen at the time the NaO_x builds in for Figure 3-4 (800s), is not modeled in MELCOR and thus could not be captured.

3.2.2.4.1. Two-cell Mixing The mixing of aerosol species in the containment atmosphere was experimentally determined to be poor during the spray periods of Na and NaI. This resulted in a two cell formation (see Figure 3-5) where the split was determined to be at the elevation of both the NaI spray nozzle and the Na spray nozzle (depending on whether we are tracking NaI or NaO_x species). The upper region is thought to be locally mixed through buoyancy effects that are induced through atmospheric heating of the combustion reactions of Na while the colder air in the lower cell had no measurable ability to mix with the upper cell. Thus, a weighted average was assumed for measured suspended aerosols in the upper and lower cells, based on the volumes of each region [1]. Unlike test AB5, the Na spray rate was much lower for test AB6, resulting in less of a driving force for atmospheric mixing. This is presumed to be the likely factor for the observed two cell mixing. Note, the two cell mixing was not accounted for in either MELCOR computation.

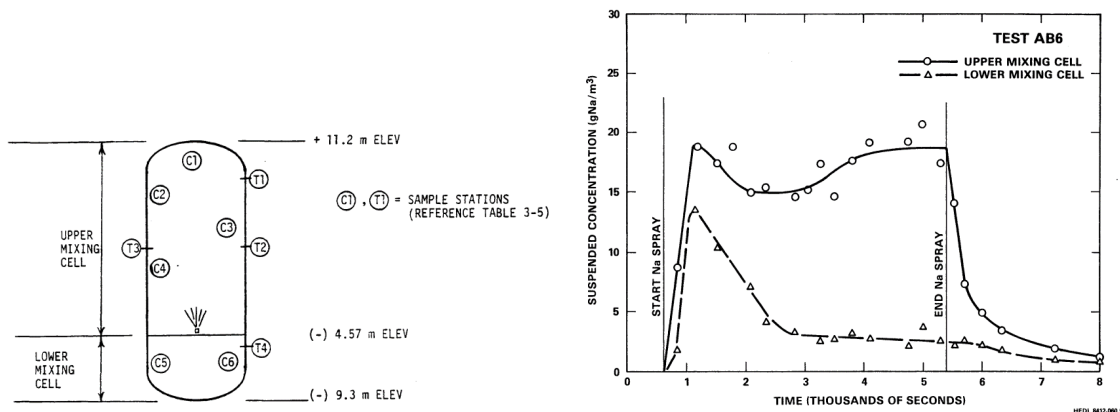


Figure 3-5 Two mixing cells in the containment atmosphere for test AB6 [1].

Despite not modeling the two-cell behavior, the suspended aerosol behavior of the NaI and NaO_x species bear agreeable predictions between computation and experiment. Note, the NaI species was injected into the system from $t=0$ s to $t=3000$ s while the molten Na was injected from $t=620$ s to $t=5400$ s (per Table 1-3). The agreement between the NaI plots using method 1 and 2 is expected since the injection method of NaI into the system using the RN class is identical. The more gratifying results are those showcasing the generation of the suspended NaO_x species. The results of method 2 are virtually identical to those using method 1, giving confidence in Na combustion reaction modeling done with the NAC package. The under/over-prediction of MELCOR to experimental data for the NaI/ NaO_x species is presumed to be attributed to the arbitrary weighting metrics used by the AB6 test group. Figure 3-6 shows the substantial difference in the measured suspended concentrations of Na in the upper and lower cells. Given variations in the chosen weighted average of the upper/lower cells toward more attribution to the upper cell would yield more agreeable experimental results to those determined using MELCOR. Re-suspension of the NaI particulates due to the Na combustion is also hypothesized as a means for the disagreement between MELCOR's predictions beyond 4000s [3] as the re-suspension of NaI was not modeled in either MELCOR computation.

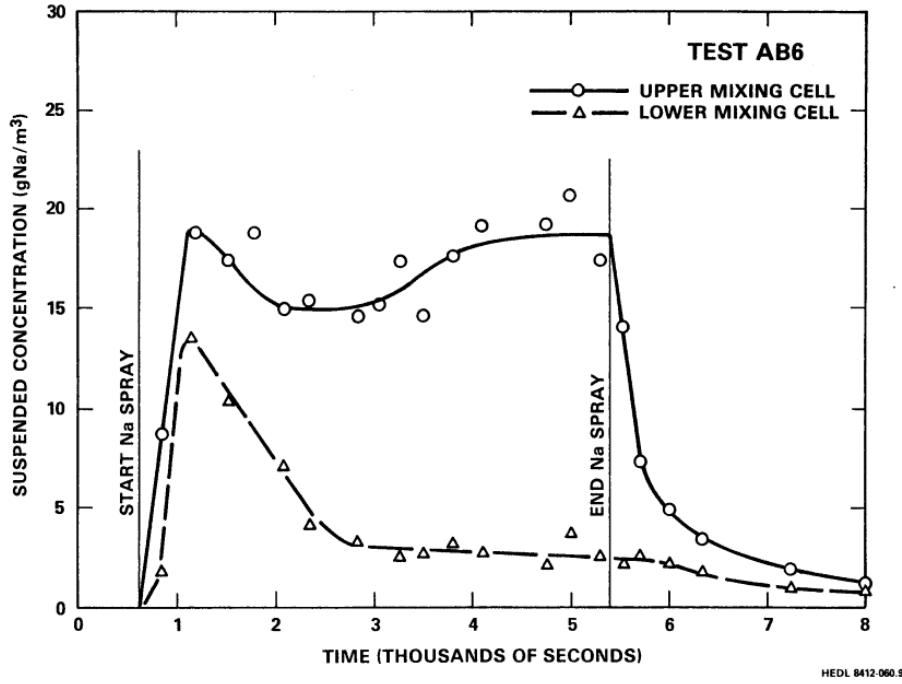


Figure 3-6 Two cell mixing plot for test AB6 [1].

3.2.3. Energy Generation & Dissipation

3.2.3.1. Combustion Mechanism To determine the amount of energy to add to the system, the model employing method 1 relies on the calculation of the energy released during the following chemical reactions found in Eq 3 and Eq 4. The total energy released from each these reactions, given as Q_1 and Q_2 , respectively, are as follows:

$$Q_1 = \left(\frac{0.9 \cdot (204.7 \times 10^3 g)}{2 \cdot (22.99 \frac{g}{mol})} \right) \cdot \left(124 \frac{kcal}{mol} \right) \cdot \left(4.184 \times 10^3 \frac{J}{kcal} \right) \quad (9)$$

$$Q_2 = \left(\frac{0.1 \cdot (204.7 \times 10^3 g)}{2 \cdot (22.99 \frac{g}{mol})} \right) \cdot \left(85 \frac{kcal}{mol} \right) \cdot \left(4.184 \times 10^3 \frac{J}{kcal} \right) \quad (10)$$

Using the same ratios of $Na_2O_2:NaOH$ produced as Souto [3], 60%/40%, Q_1 yields a value of 1.386GJ while Q_2 yields a value of 0.633 GJ. The sum of the energy output by these reactions equals 2.019 GJ. Using the ratios found after analysis of the model using method 2, 91% Na_2O_2 to 9% NaOH, yields 2.102 GJ and 0.142 GJ, respectively, yielding approximately 2.24 GJ. Outputting the plot parameter for energy added to the atmosphere yielded a value of 2.22GJ. This was found to be good agreement between theoretical calculations used both on paper and within the model itself. This also highlights an oversight of Souto's model/work where they imported more energy (+30%) than the system would have generated otherwise by using the test AB5 values instead of calculating new values using 204.7kg rather than 223kg. Furthermore, discrepancies are noted within the original AB6 report output [1] where Table 4-2 highlights their energy balance. This table shows a heat generated by chemical reaction as having a value of

2.86GJ. This number cannot be reasonably achieved even through the singular formation of Na_2O_2 , the reaction producing more energy. It is not clear where this number came from, but it is clear that it is incorrect nonetheless and could be suffering from the same issues as Souto, assuming the same input mass (223 kg Na from test AB5 $\neq$ 204.7 kg Na from test AB6) and aerosol formation (60% Na_2O_2 , 40% NaOH). In addition, Souto's work does not account for the amount of N_2 gas pumped into the system through the release of NaI. Over the course of 0 to 3000s, N_2 was injected into the CSTF at a rate of 0.018 kg/s yielding 53 kg of additional gas. Adding this to Souto's analysis would yield an increase in pressure, likely meeting an identical response to the outputs from method 2. Overall, the results of modeling AB6 using method 2 gave much more agreeable results pertaining to energy generation and energy dissipation than test AB5.

3.2.3.2. Thermal-hydraulic Response Figure 3-7 below compares the temperature and pressure plots between method 1, 2 and the experimental data.

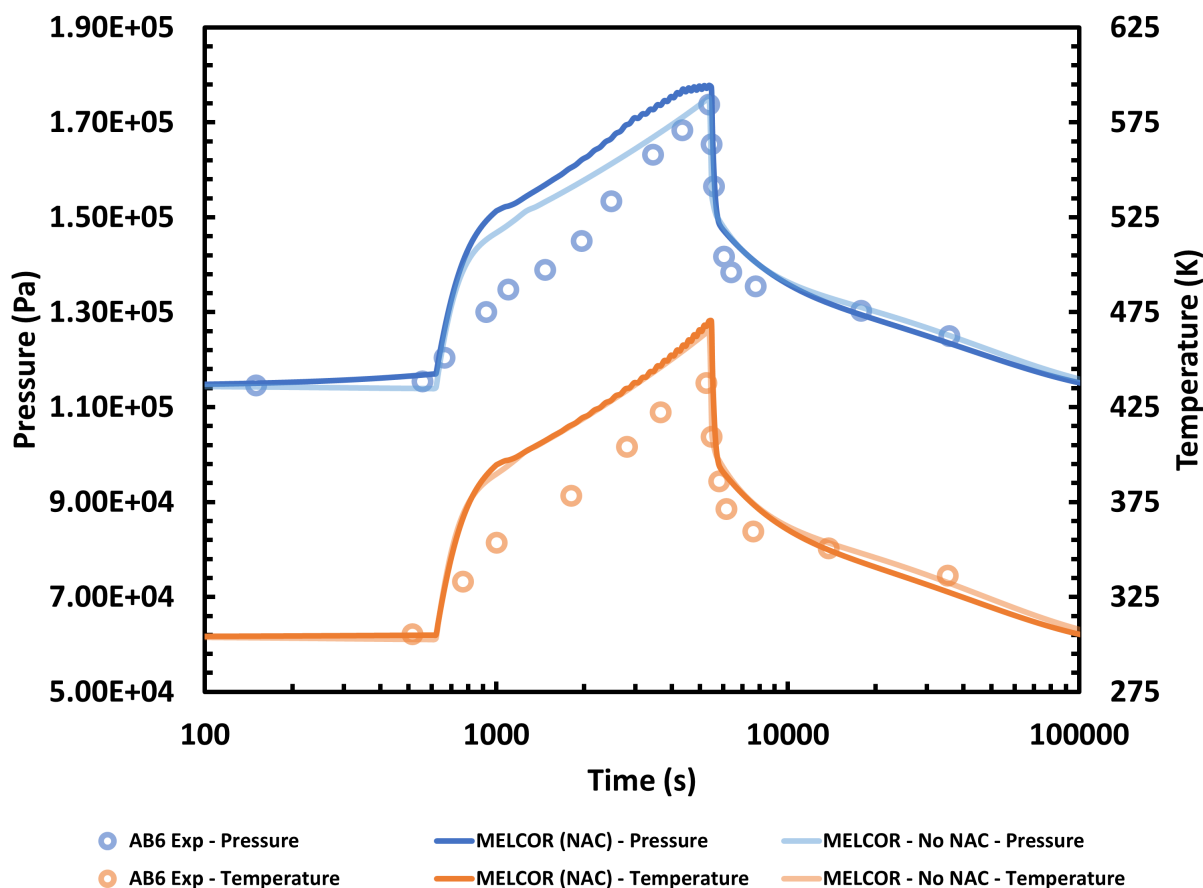


Figure 3-7 Pressure/Temperature plots for the AB6 test.

There is generally good agreement between models running method 1, 2 and experimental data for the thermal-hydraulic response of the system. The models running method 2 are found to be

properly accounting for the amount of heat input into the system, unlike test AB5 which showcased an excess temperature and pressure spike in the system. The minor overestimation in temperature can be attributed to the lack of radiative heat transfer from the combustion flame to the heat structures. The lack of heat capacity for the sodium aerosol mass may also be a contributor to early discrepancies. The effects of radiative heat transfer are hypothesized to be far less exaggerated in AB6 than in AB5 due to the extended Na spray period (4800 seconds vs. 872 seconds) for roughly the same amount of molten Na (204 kg vs. 223 kg). Given the direct removal of 35% of the heat from combustion, it is postulated that the rise in temperature and pressure of the system would become as gradual as the experimental results depict.

4. CONCLUSION

The NAC package needs some improvements in temperature, pressure and overall energy transfer modeling. The results highlight a need for the ability to capture the effects of fire radiative heat transfer. NAC also needs to be able to define fractionation of NaOH in addition to Na_2O_2 and Na_2O for sodium spray fire scenarios in which humidity or moisture is present in the air. The volume mean sodium droplet diameter, DME, was a primarily sensitive and significant variable that was found for the runs using method 2 in weighting the temperature, pressure and aerosol generation as the size of the spray droplets heavily drives combustion rates and completeness.

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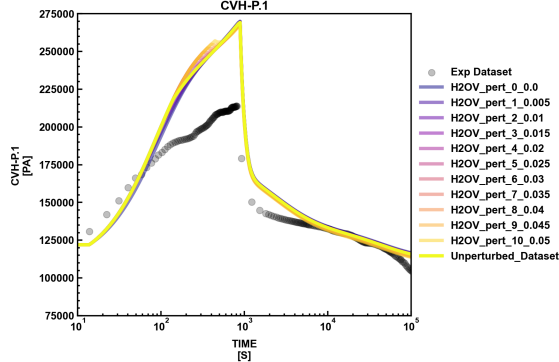
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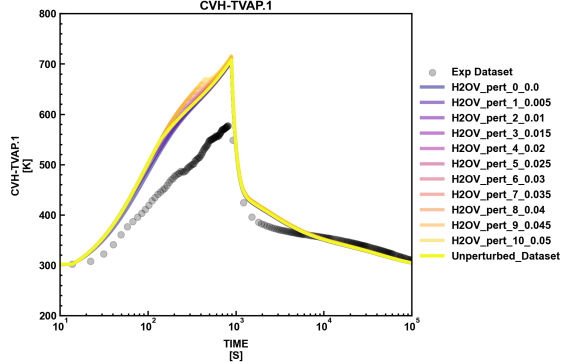
APPENDIX A. AB5: SELECT PARAMETER PERTURBATIONS

A.1. NCG_INPUT

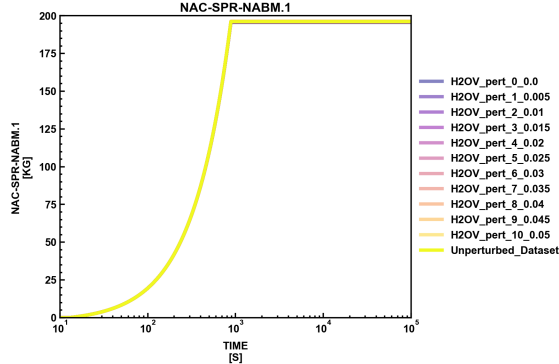
A.1.1. H2OV



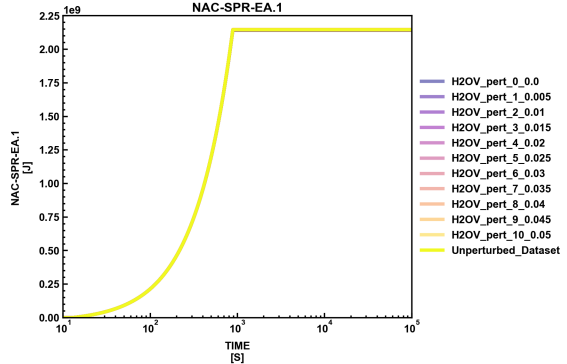
(a) Pressure



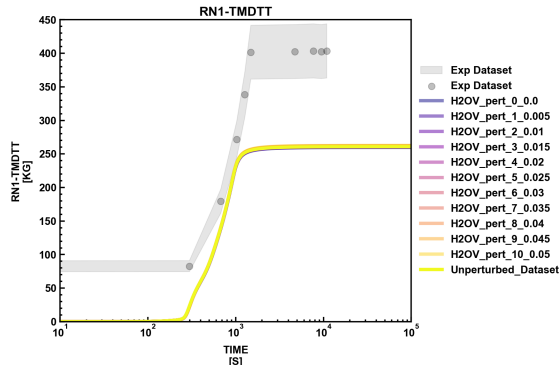
(b) Atmospheric Temperature



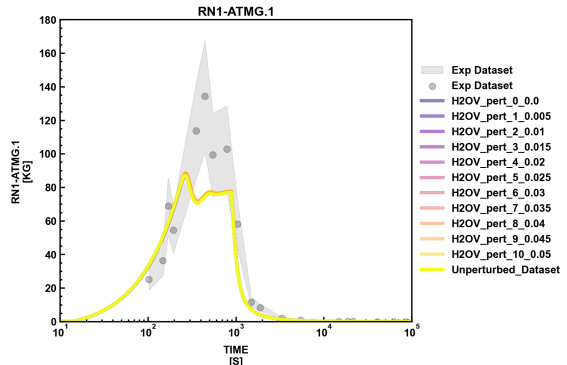
(c) Burned Sodium Mass



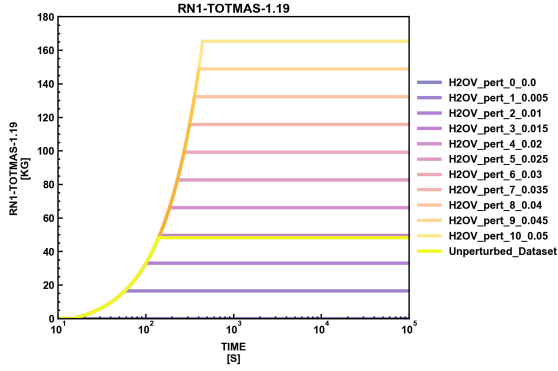
(d) Energy Input to Atmosphere



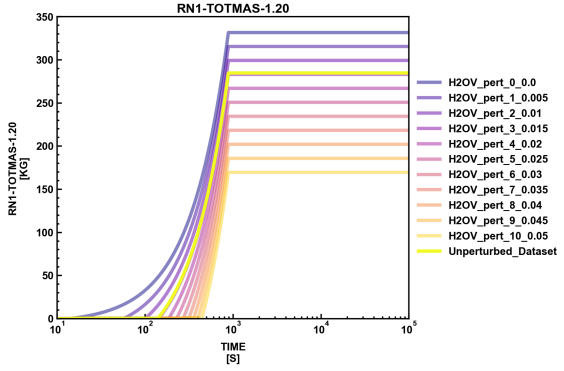
(e) Total Mass Deposited



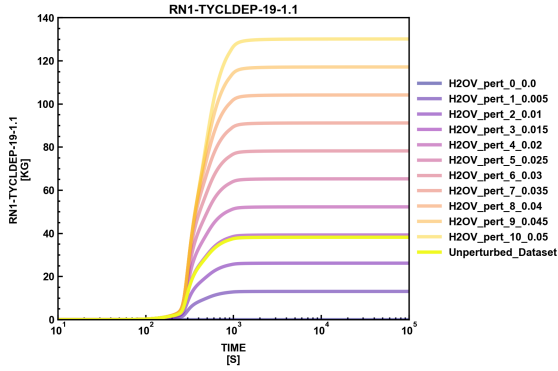
(f) Total Suspended Aerosol Mass



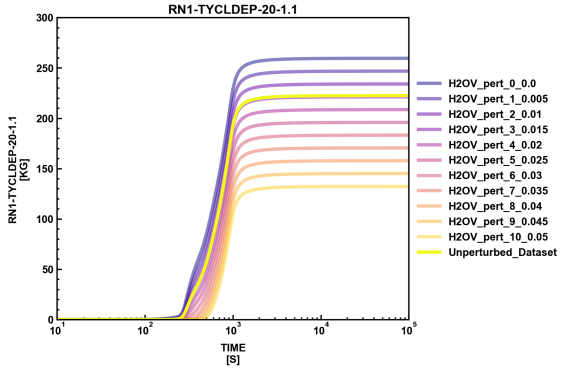
(g) Total Mass, NaOH



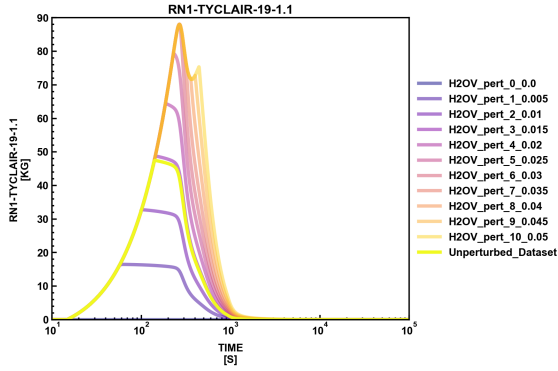
(h) Total Mass, Na₂O₂



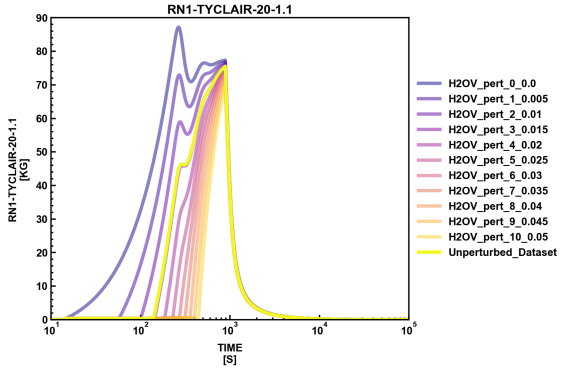
(i) Deposited Mass, NaOH



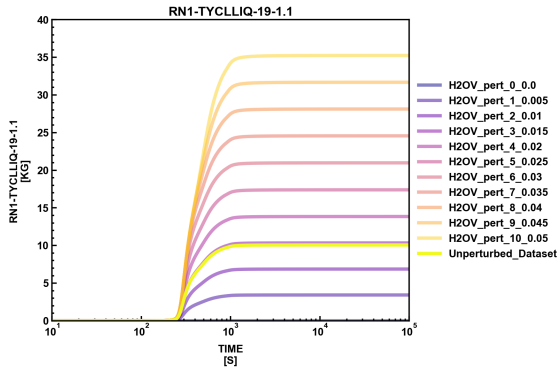
(j) Deposited Mass, Na₂O₂



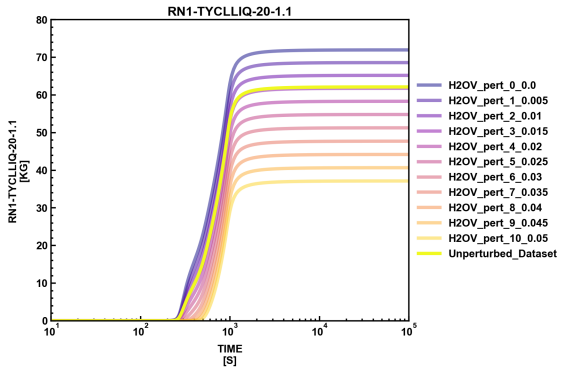
(k) Suspended Mass, NaOH



(l) Suspended Mass, Na₂O₂



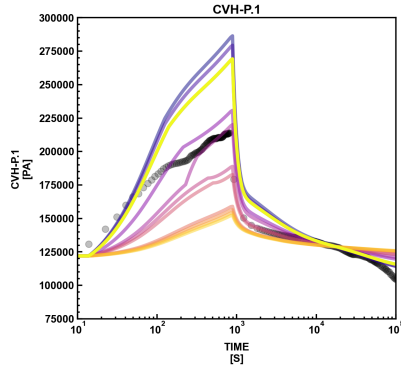
(m) Pool Mass, NaOH



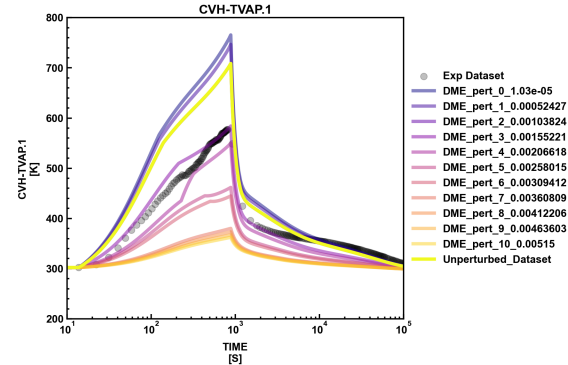
(n) Pool Mass, Na₂O₂

A.2. NAC_INPUT

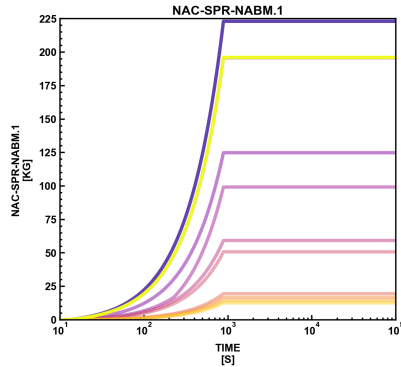
A.2.1. DME



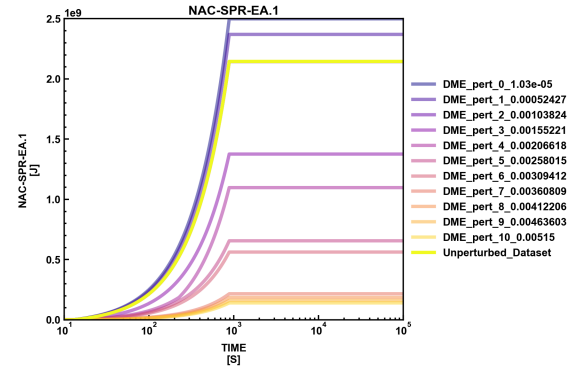
(a) Pressure



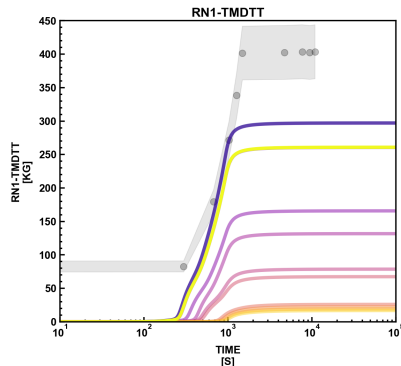
(b) Atmospheric Temperature



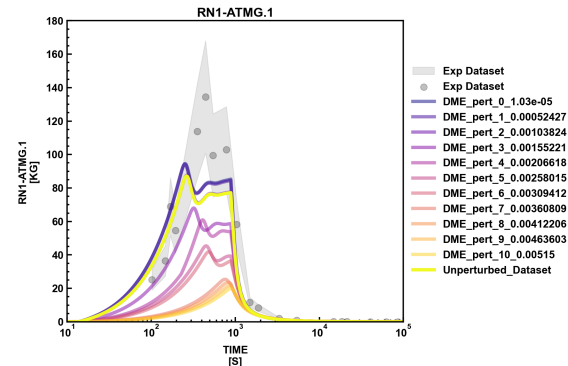
(c) Burned Sodium Mass



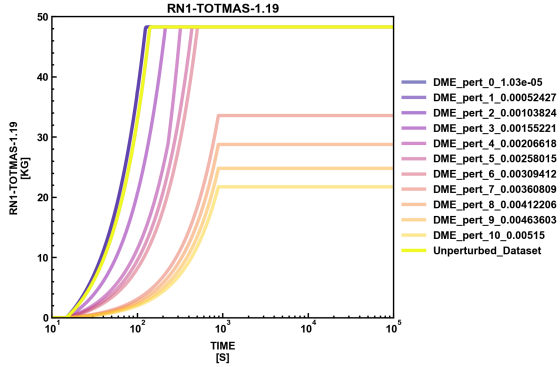
(d) Energy Input to Atmosphere



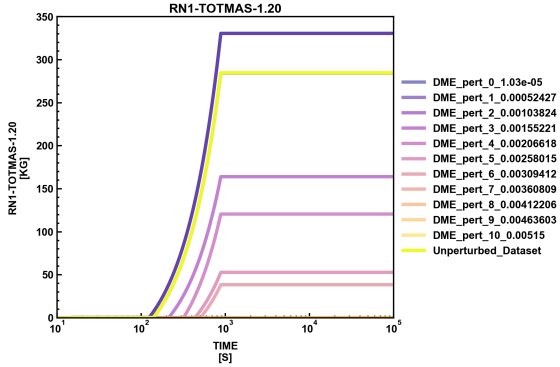
(e) Total Mass Deposited



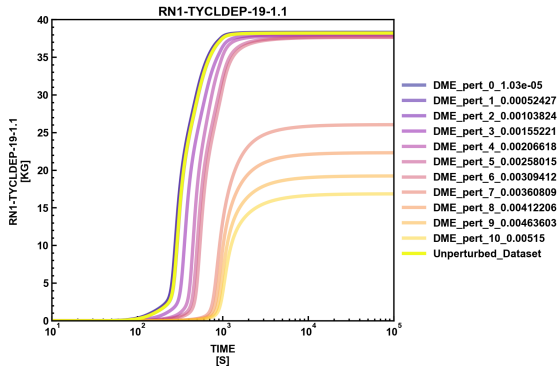
(f) Total Suspended Aerosol Mass



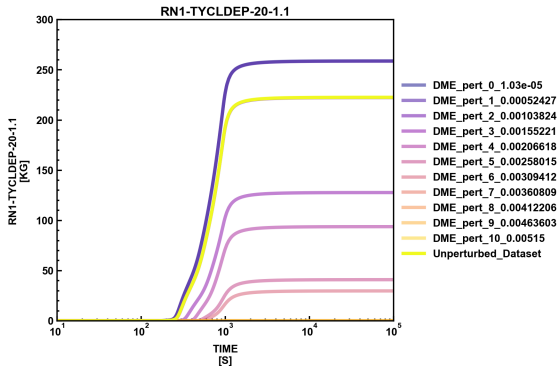
(g) Total Mass, NaOH



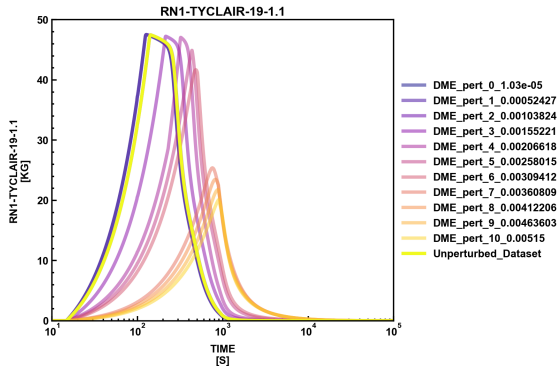
(h) Total Mass, Na₂O₂



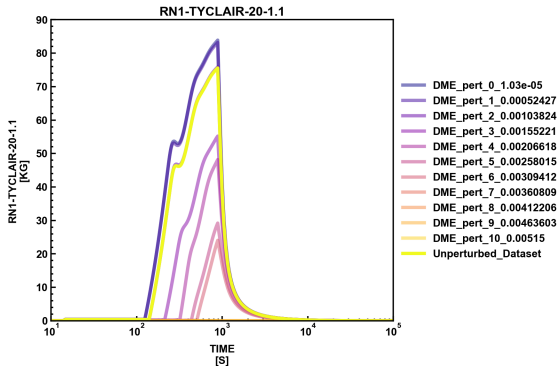
(i) Deposited Mass, NaOH



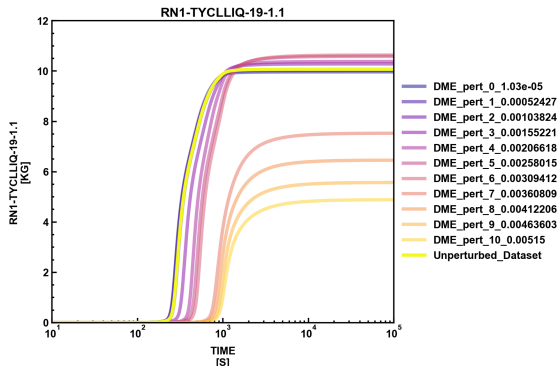
(j) Deposited Mass, Na₂O₂



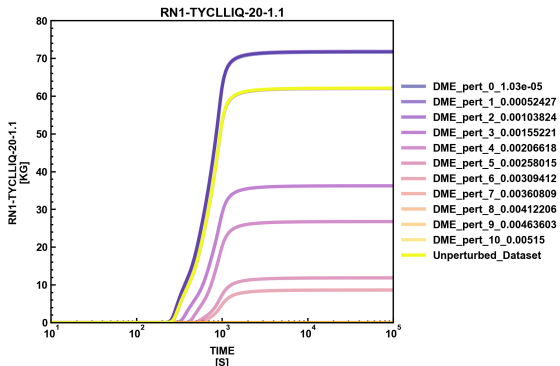
(k) Suspended Mass, NaOH



(l) Suspended Mass, Na₂O₂

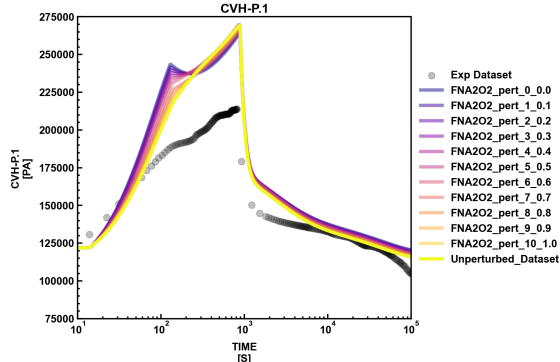


(m) Pool Mass, NaOH

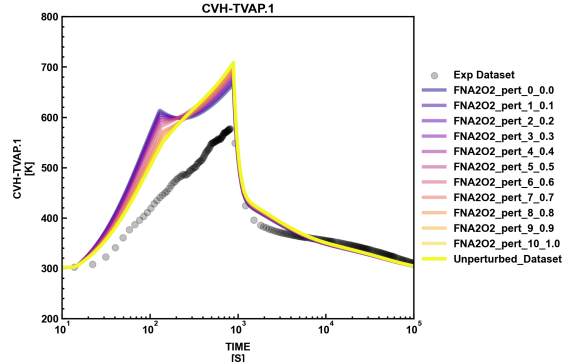


(n) Pool Mass, Na₂O₂

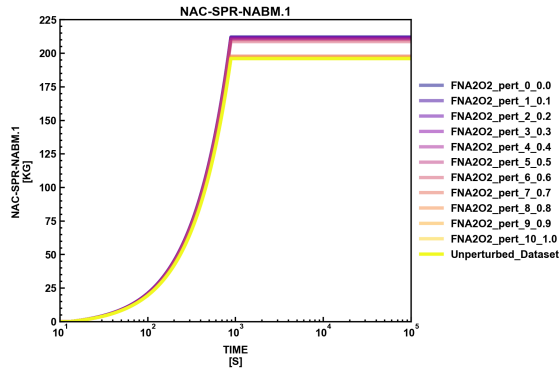
A.2.2. FNA202



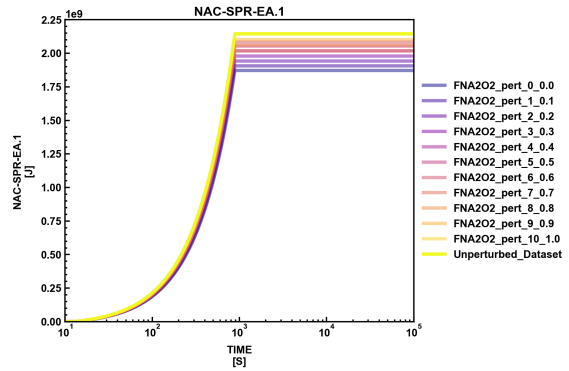
(a) Pressure



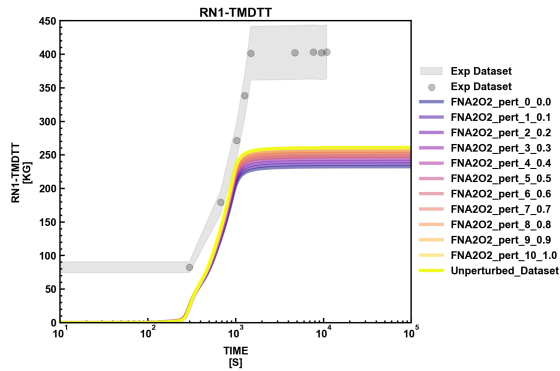
(b) Atmospheric Temperature



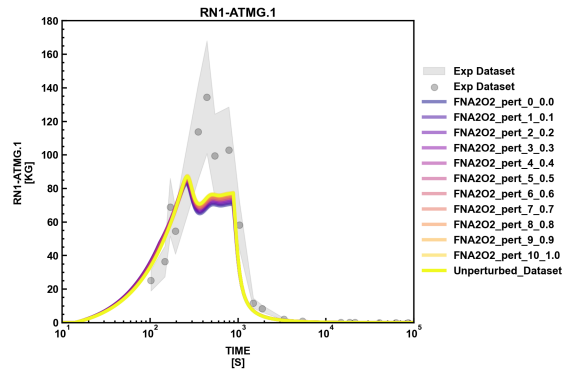
(c) Burned Sodium Mass



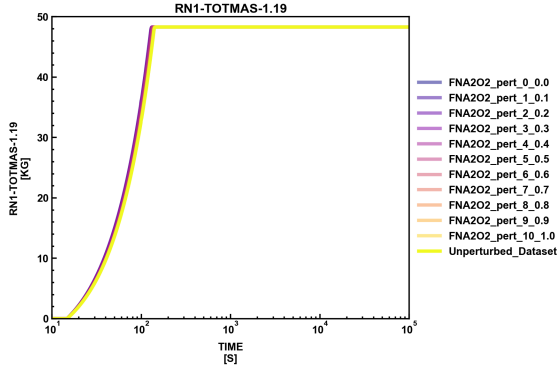
(d) Energy Input to Atmosphere



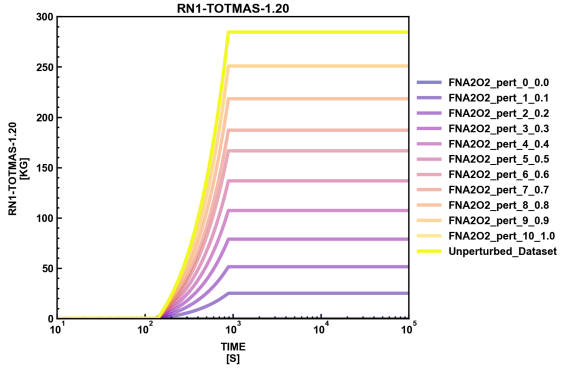
(e) Total Mass Deposited



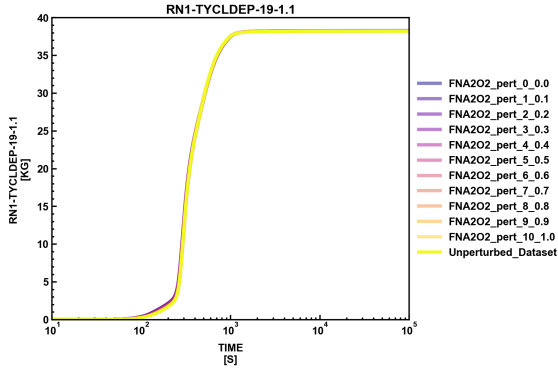
(f) Total Suspended Aerosol Mass



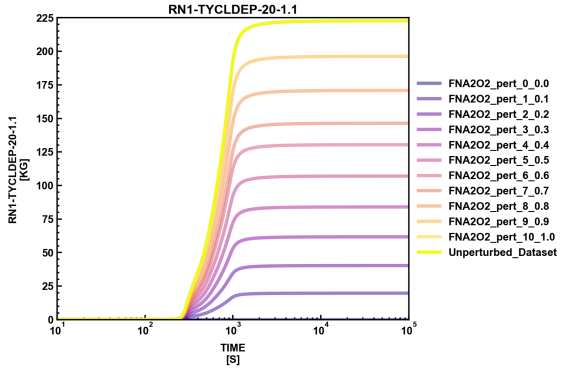
(g) Total Mass, NaOH



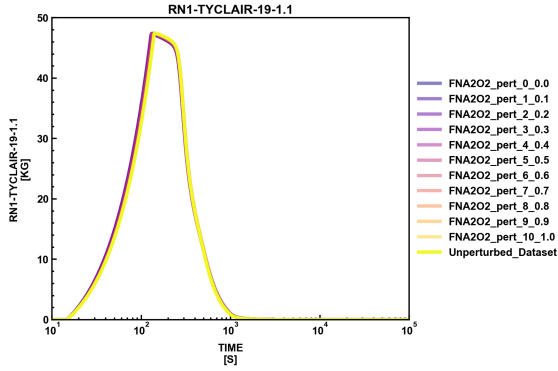
(h) Total Mass, Na_2O_2



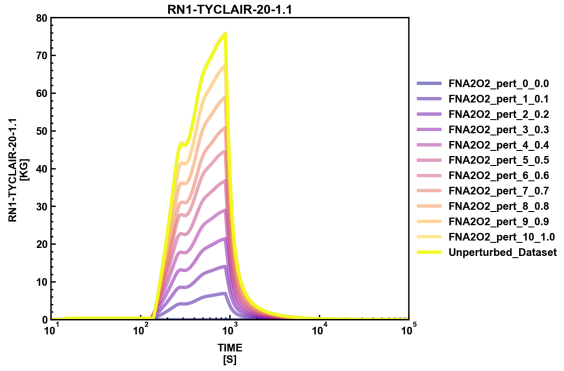
(i) Deposited Mass, NaOH



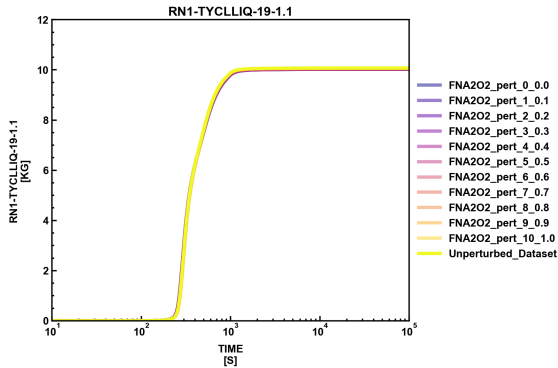
(j) Deposited Mass, Na_2O_2



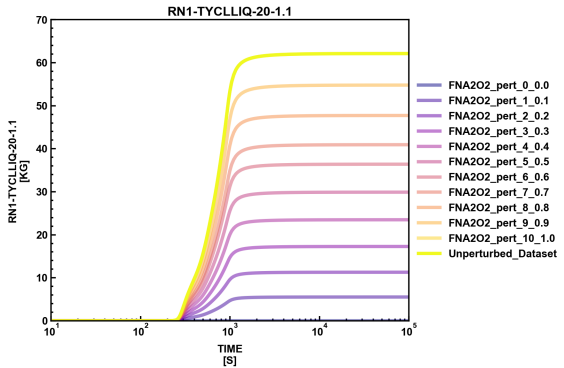
(k) Suspended Mass, NaOH



(l) Suspended Mass, Na_2O_2

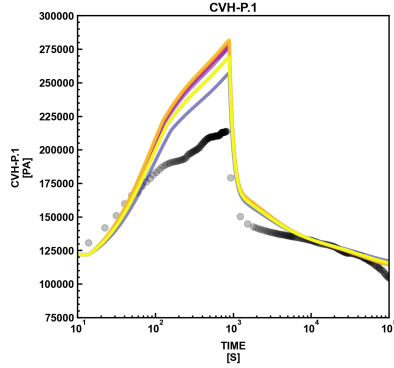


(m) Pool Mass, NaOH

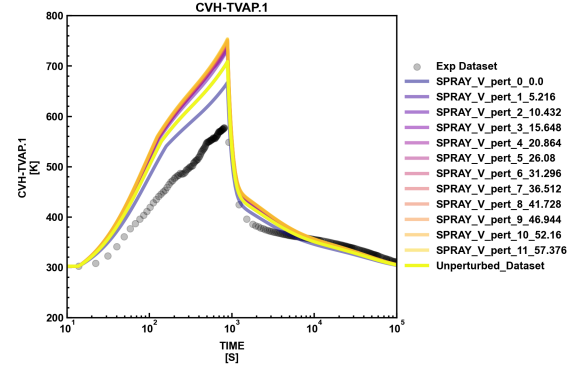


(n) Pool Mass, Na_2O_2

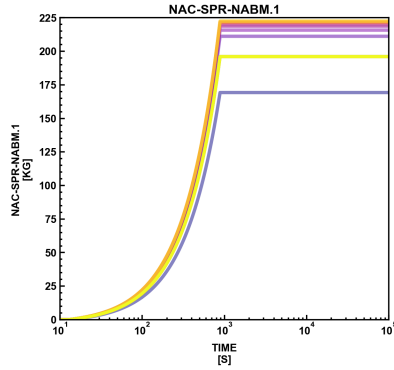
A.2.3. SPRAY_V



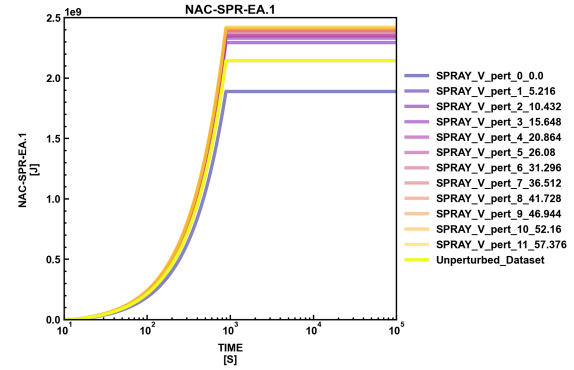
(a) Pressure



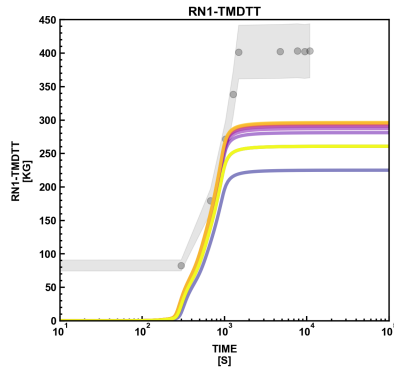
(b) Atmospheric Temperature



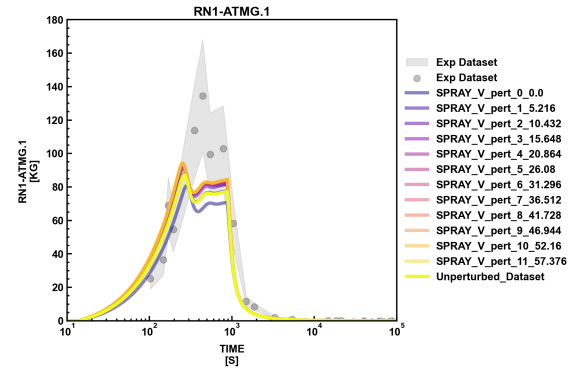
(c) Burned Sodium Mass



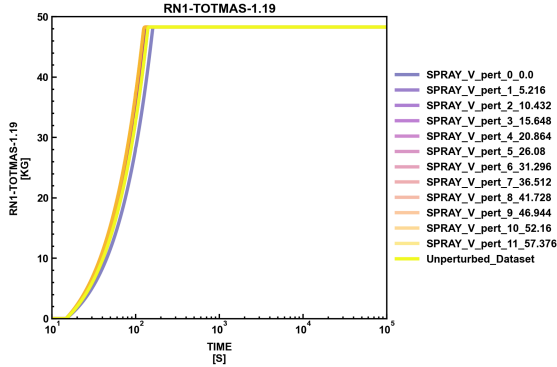
(d) Energy Input to Atmosphere



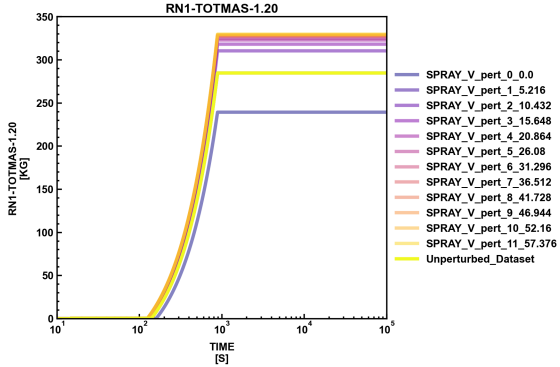
(e) Total Mass Deposited



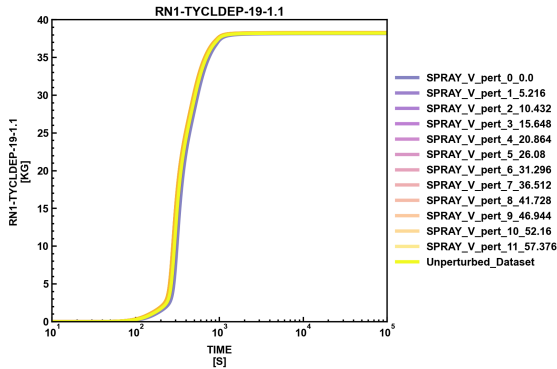
(f) Total Suspended Aerosol Mass



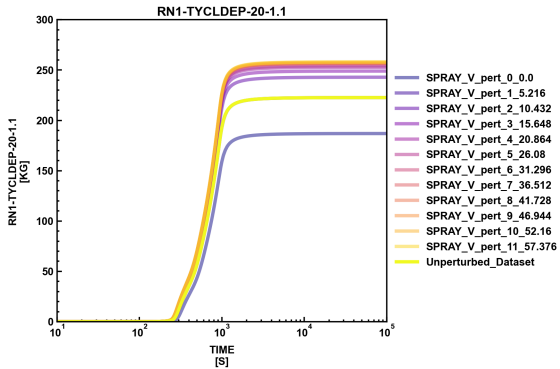
(g) Total Mass, NaOH



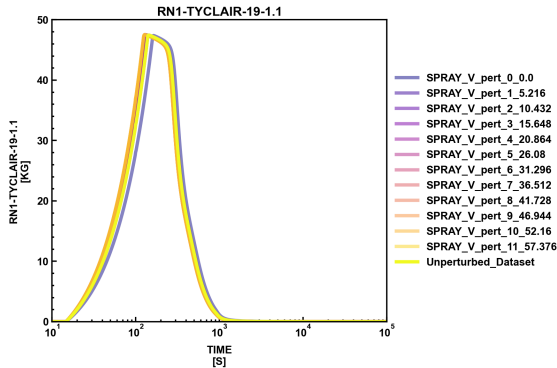
(h) Total Mass, Na₂O₂



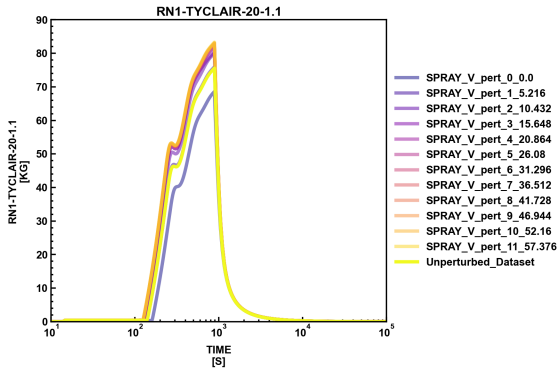
(i) Deposited Mass, NaOH



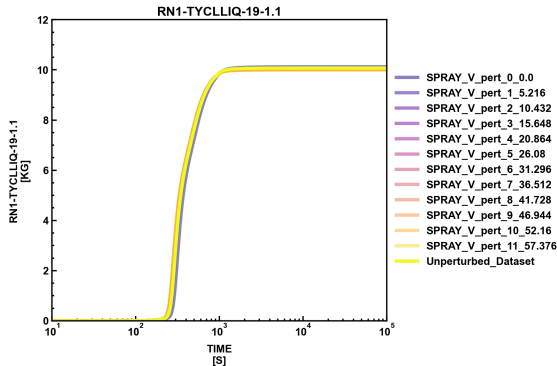
(j) Deposited Mass, Na₂O₂



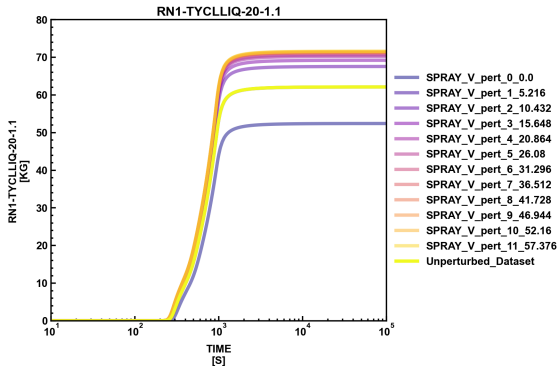
(k) Suspended Mass, NaOH



(l) Suspended Mass, Na₂O₂



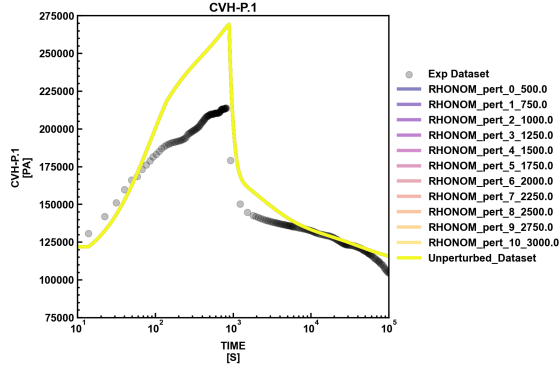
(m) Pool Mass, NaOH



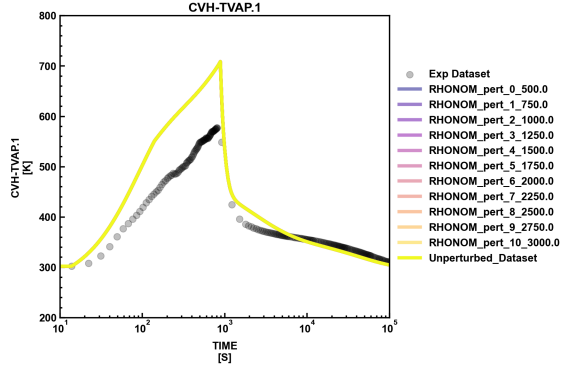
(n) Pool Mass, Na₂O₂

A.3. RN1_INPUT

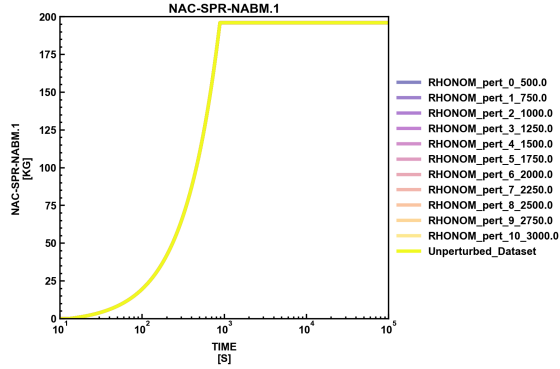
A.3.1. RHONOM



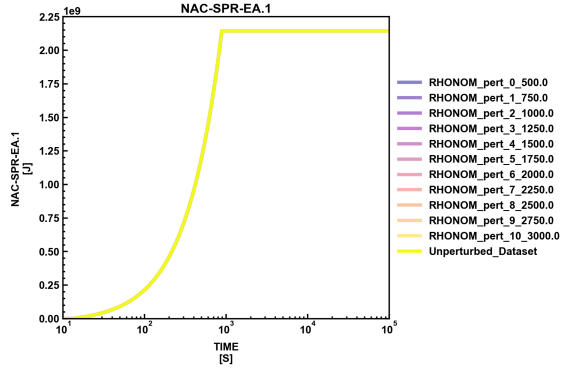
(a) Pressure



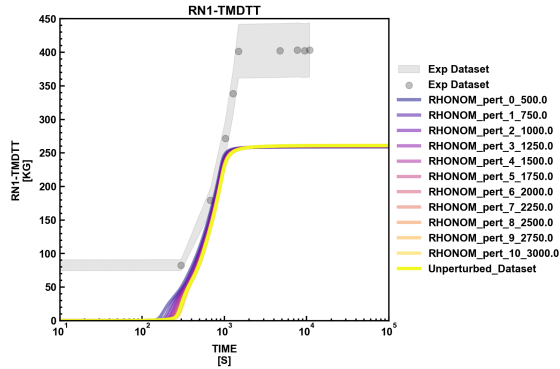
(b) Atmospheric Temperature



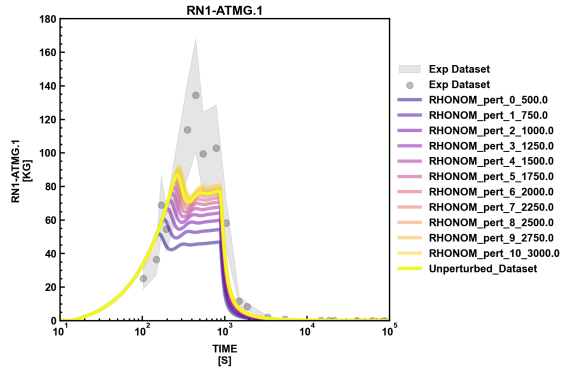
(c) Burned Sodium Mass



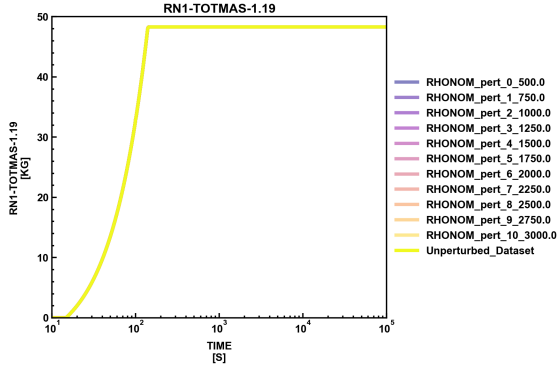
(d) Energy Input to Atmosphere



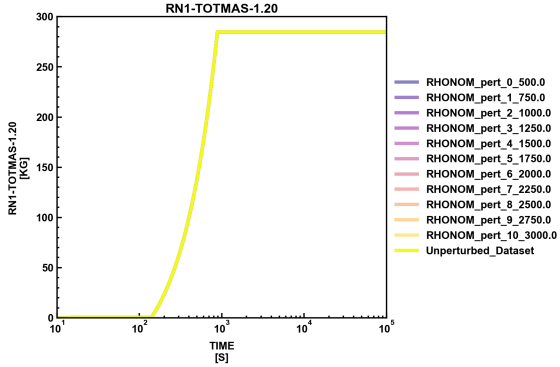
(e) Total Mass Deposited



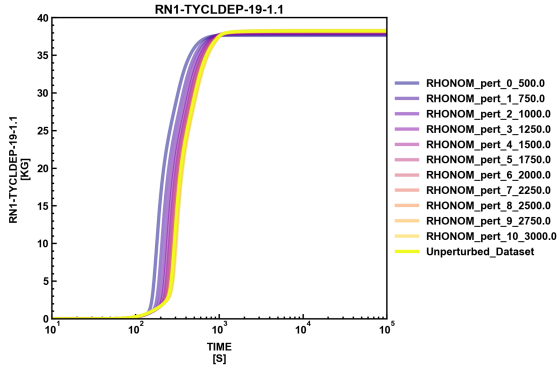
(f) Total Suspended Aerosol Mass



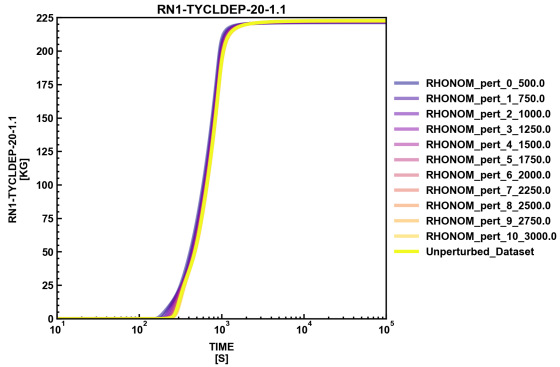
(g) Total Mass, NaOH



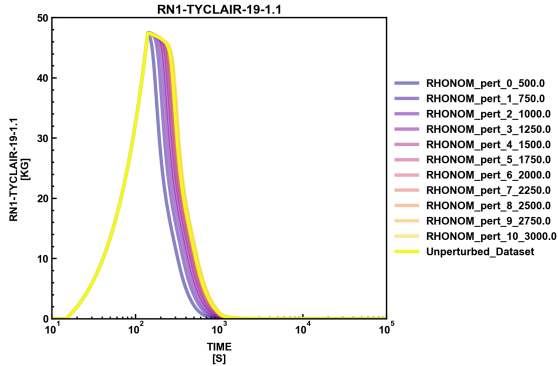
(h) Total Mass, Na₂O₂



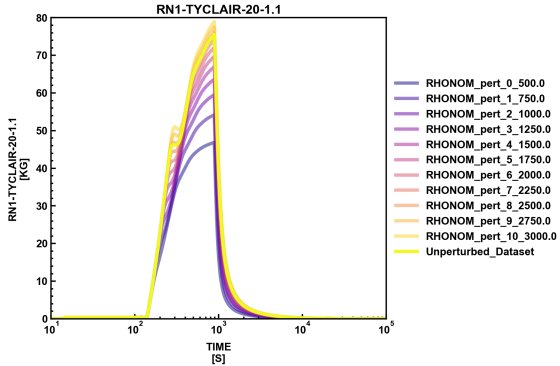
(i) Deposited Mass, NaOH



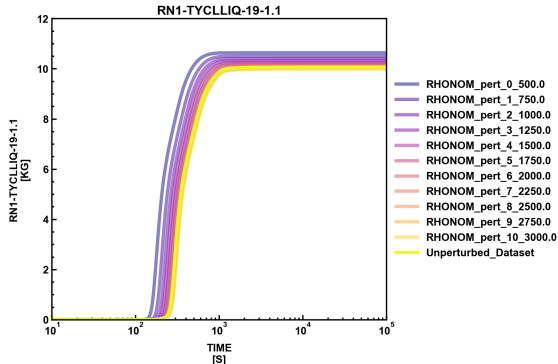
(j) Deposited Mass, Na₂O₂



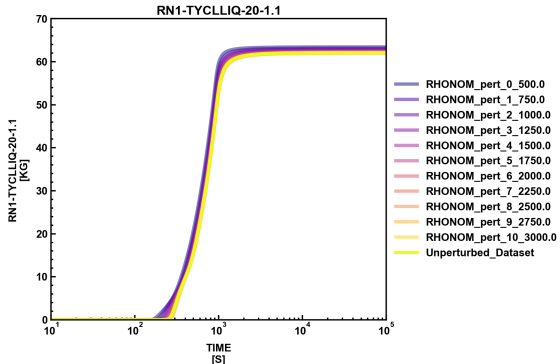
(k) Suspended Mass, NaOH



(l) Suspended Mass, Na₂O₂

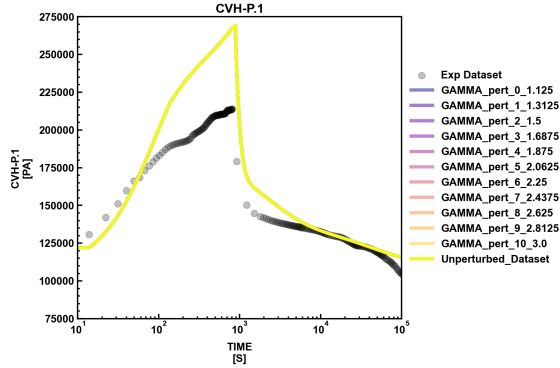


(m) Pool Mass, NaOH

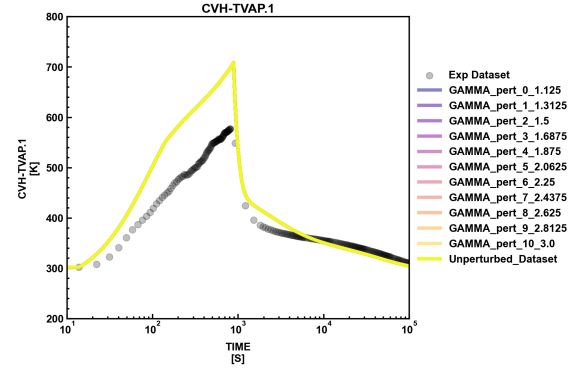


(n) Pool Mass, Na₂O₂

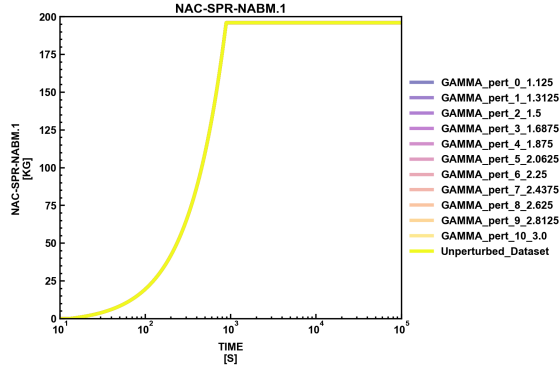
A.3.2. GAMMA



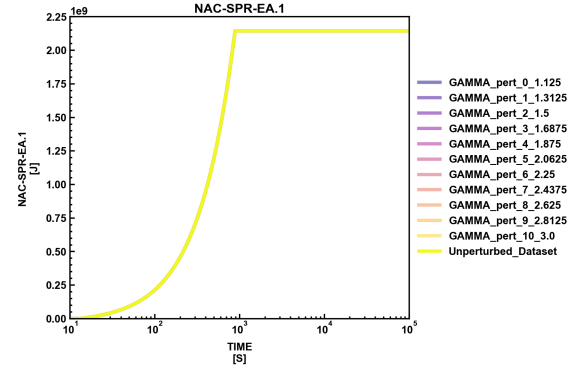
(a) Pressure



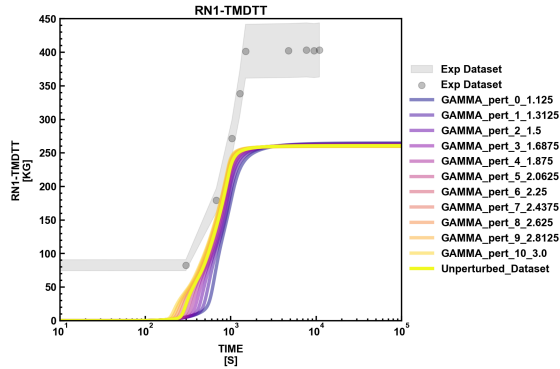
(b) Atmospheric Temperature



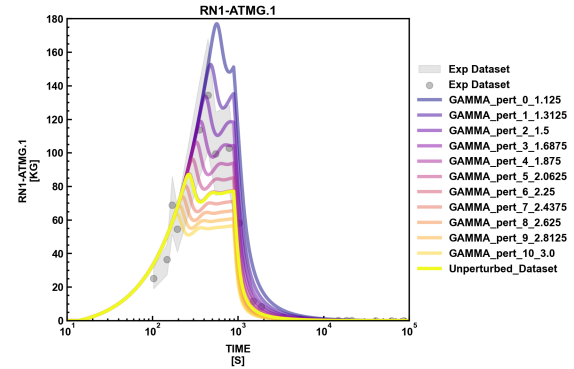
(c) Burned Sodium Mass



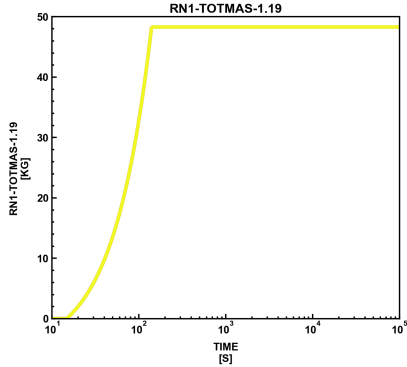
(d) Energy Input to Atmosphere



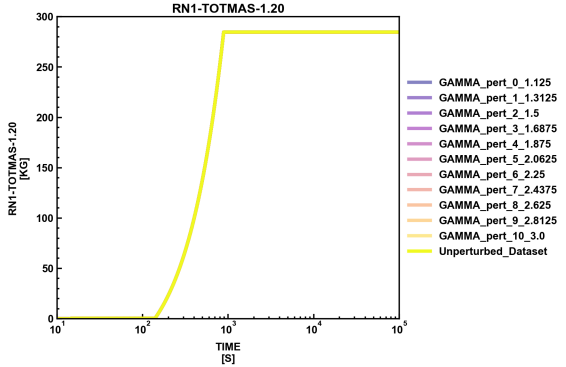
(e) Total Mass Deposited



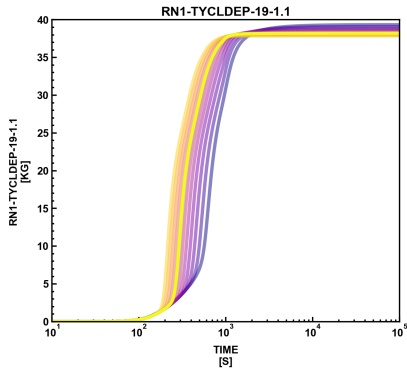
(f) Total Suspended Aerosol Mass



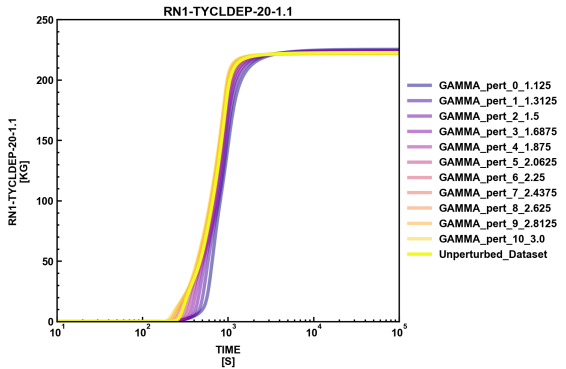
(g) Total Mass, NaOH



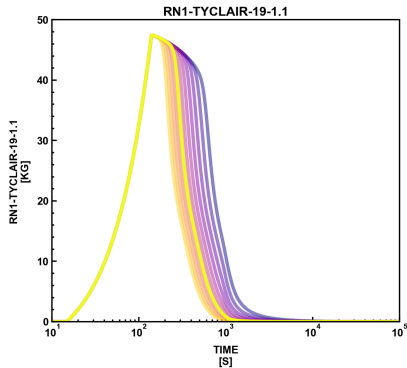
(h) Total Mass, Na₂O₂



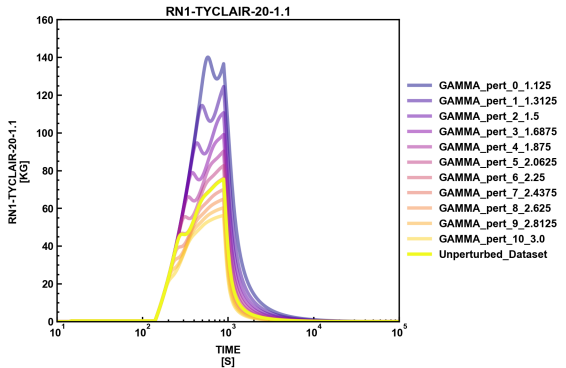
(i) Deposited Mass, NaOH



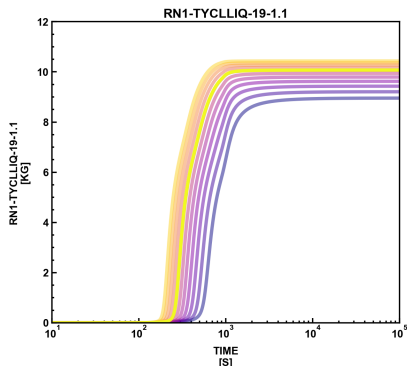
(j) Deposited Mass, Na₂O₂



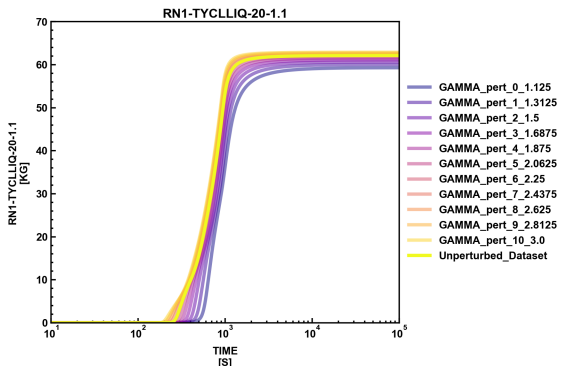
(k) Suspended Mass, NaOH



(l) Suspended Mass, Na₂O₂

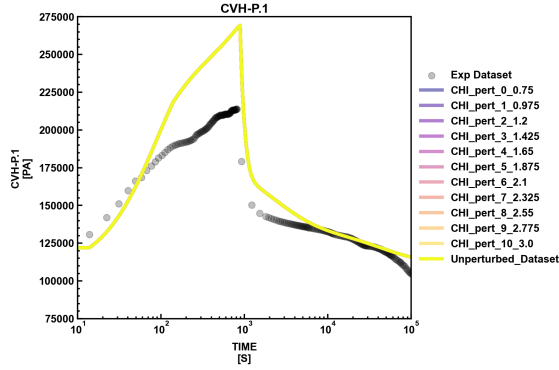


(m) Pool Mass, NaOH

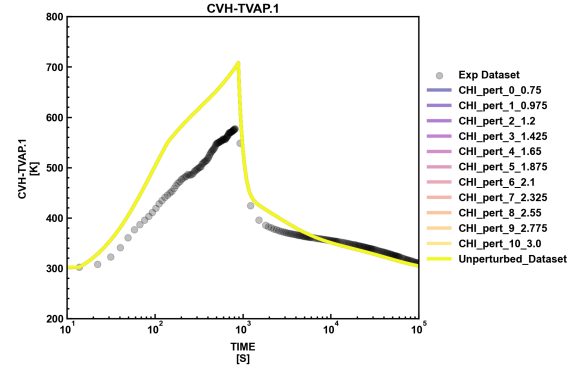


(n) Pool Mass, Na₂O₂

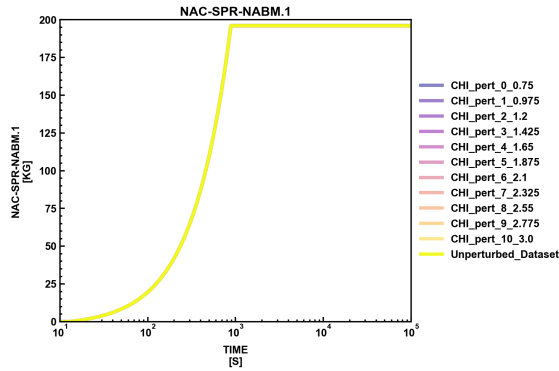
A.3.3. CHI



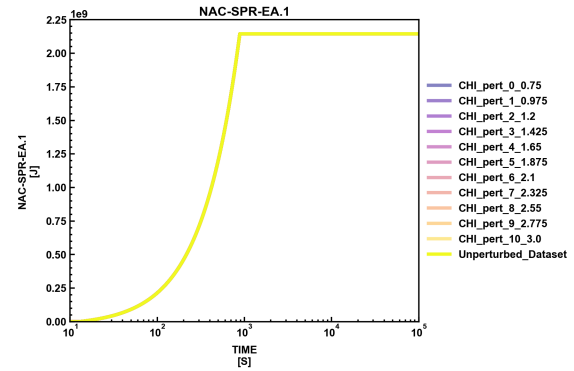
(a) Pressure



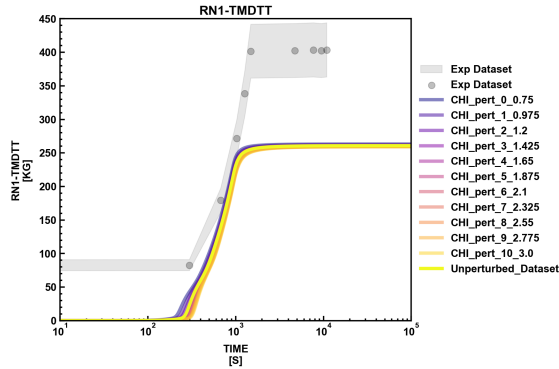
(b) Atmospheric Temperature



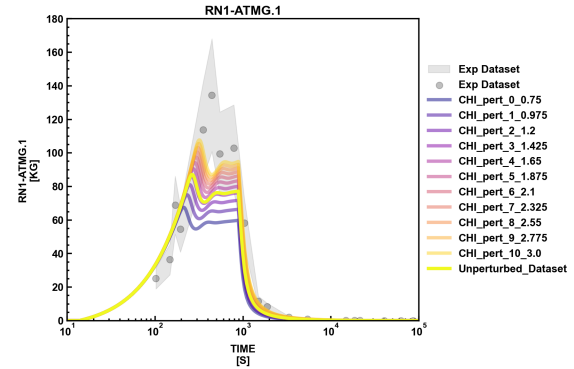
(c) Burned Sodium Mass



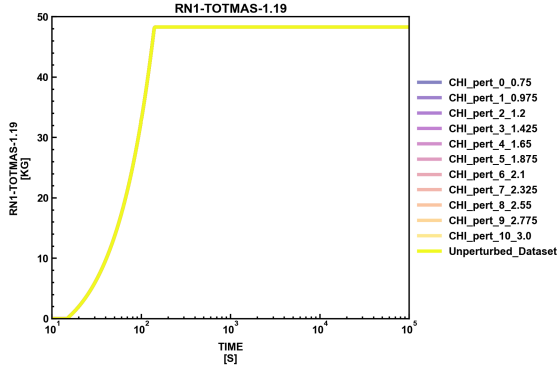
(d) Energy Input to Atmosphere



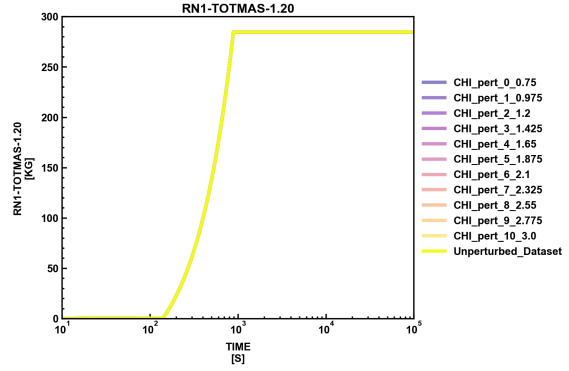
(e) Total Mass Deposited



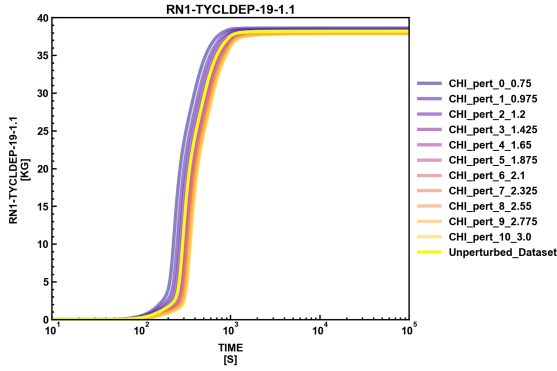
(f) Total Suspended Aerosol Mass



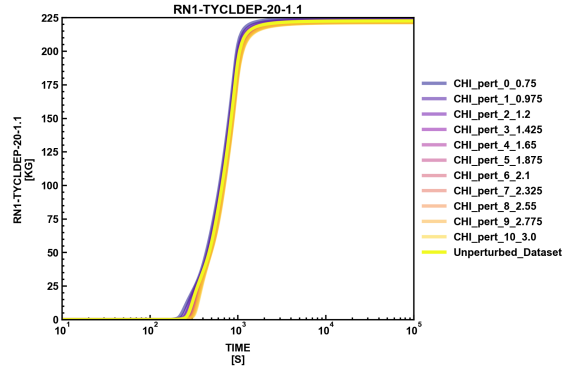
(g) Total Mass, NaOH



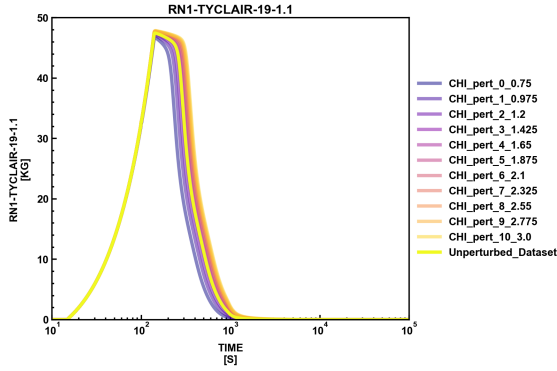
(h) Total Mass, Na₂O₂



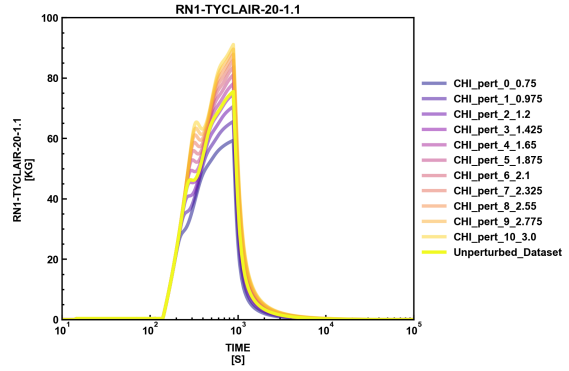
(i) Deposited Mass, NaOH



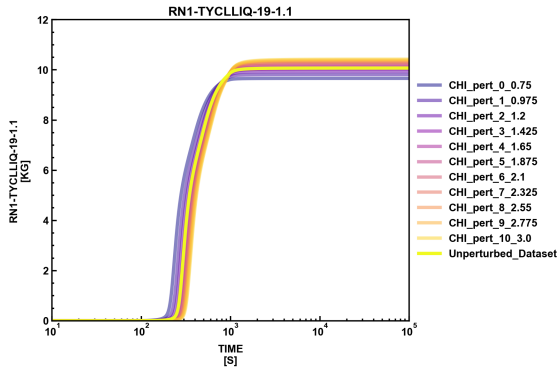
(j) Deposited Mass, Na₂O₂



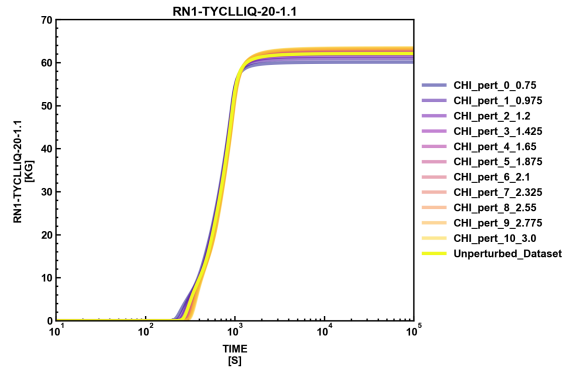
(k) Suspended Mass, NaOH



(l) Suspended Mass, Na₂O₂



(m) Pool Mass, NaOH

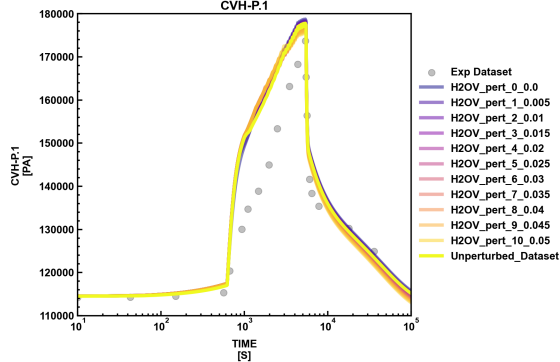


(n) Pool Mass, Na₂O₂

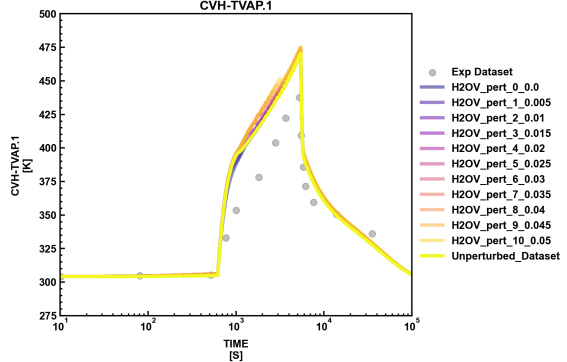
APPENDIX B. AB6: SELECT PARAMETER PERTURBATIONS

B.1. NCG_INPUT

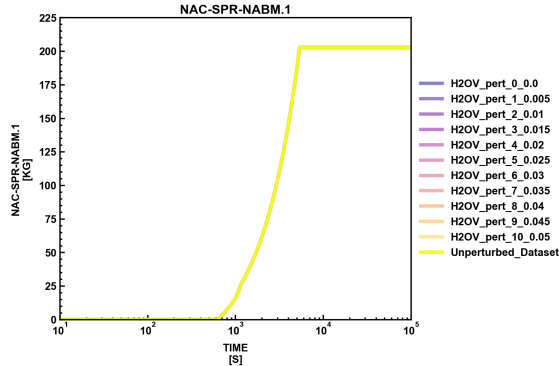
B.1.1. H2OV



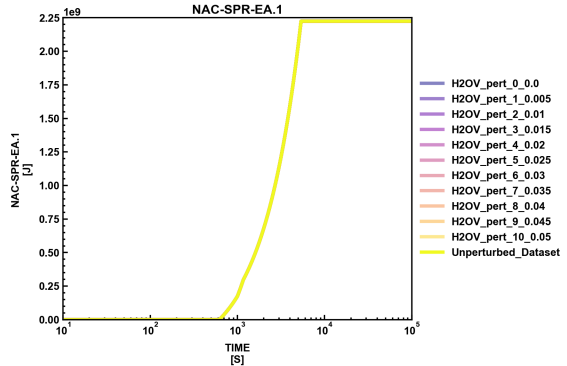
(a) Pressure



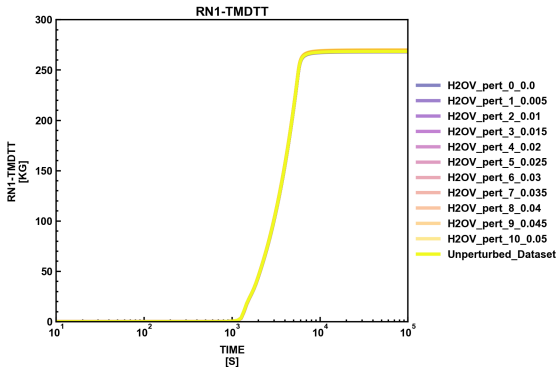
(b) Atmospheric Temperature



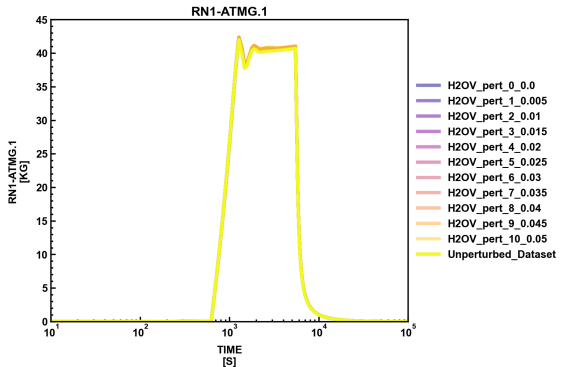
(c) Burned Sodium Mass



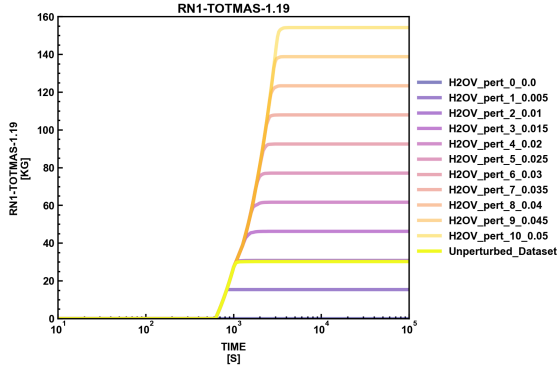
(d) Energy Input to Atmosphere



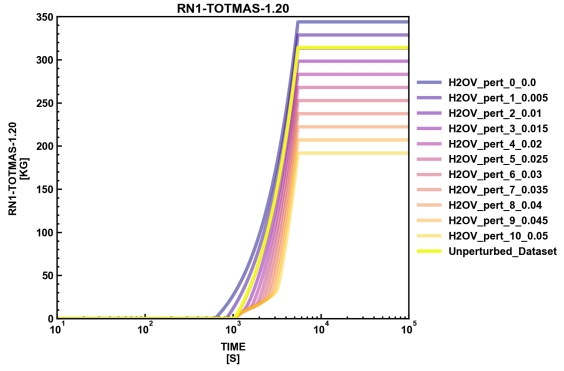
(e) Total Mass Deposited



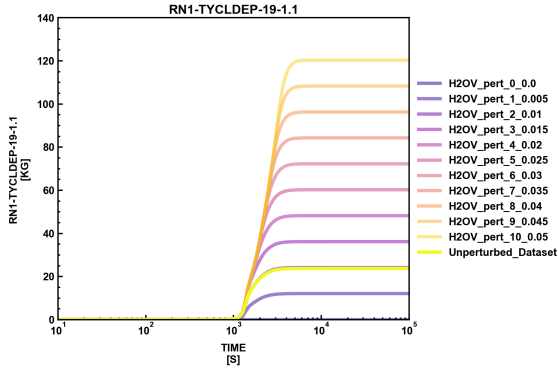
(f) Total Suspended Aerosol Mass



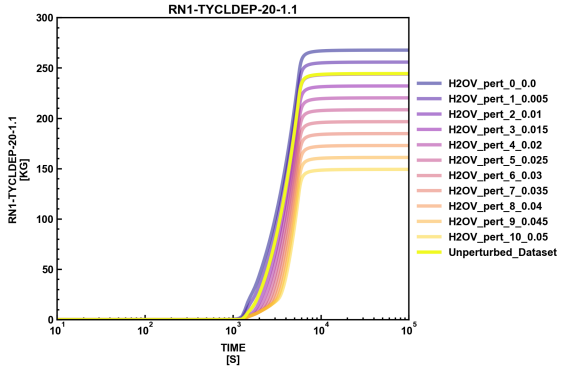
(g) Total Mass, NaOH



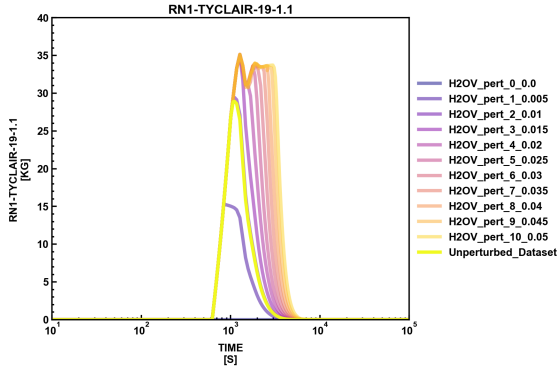
(h) Total Mass, Na₂O₂



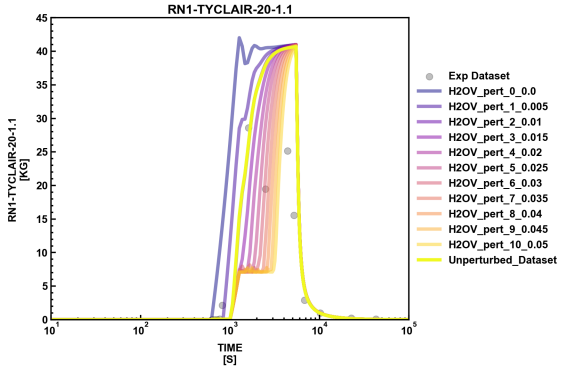
(i) Deposited Mass, NaOH



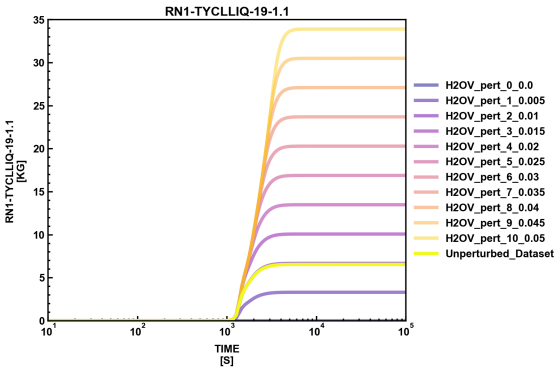
(j) Deposited Mass, Na₂O₂



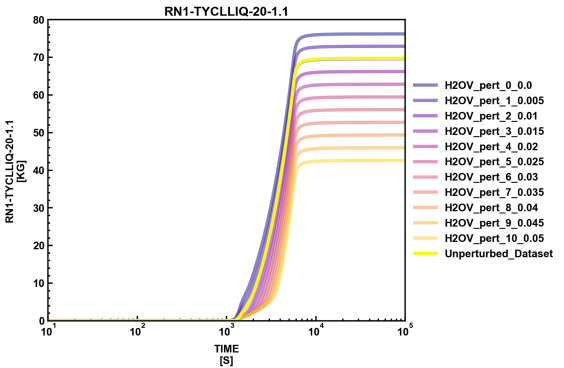
(k) Suspended Mass, NaOH



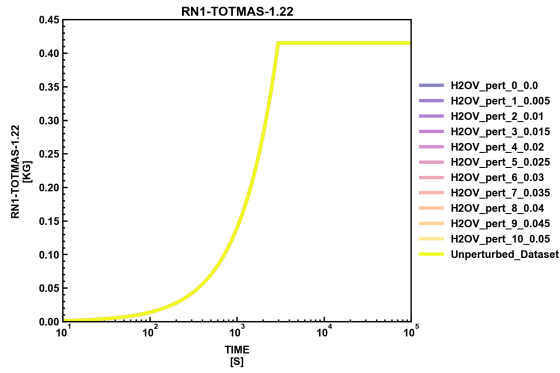
(l) Suspended Mass, Na₂O₂



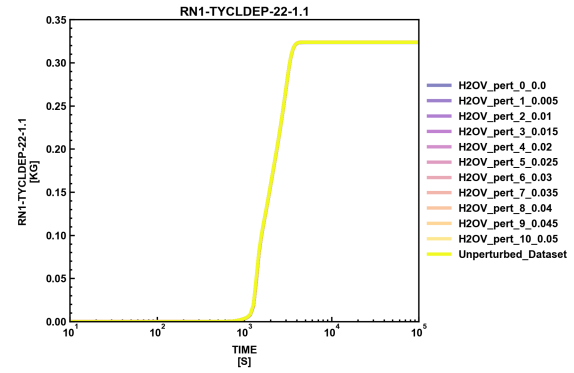
(m) Pool Mass, NaOH



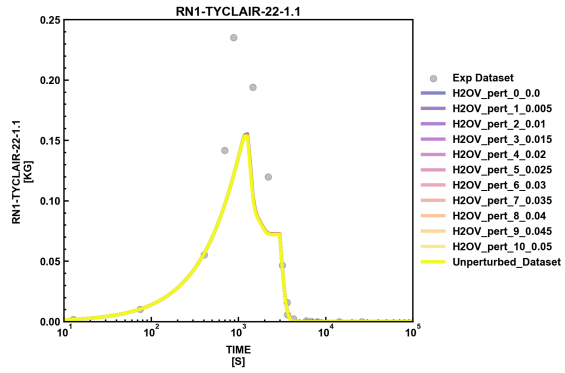
(n) Pool Mass, Na₂O₂



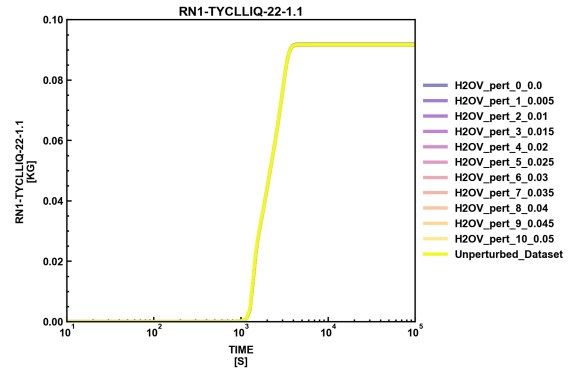
(o) Total Mass, NaI



(p) Deposited Mass, NaI



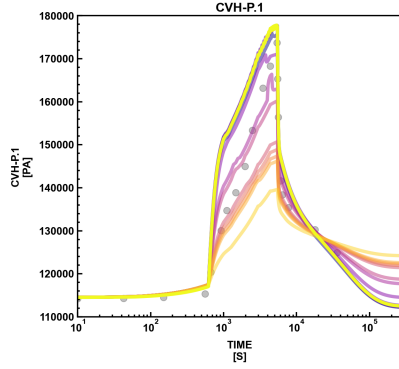
(q) Suspended Mass, NaI



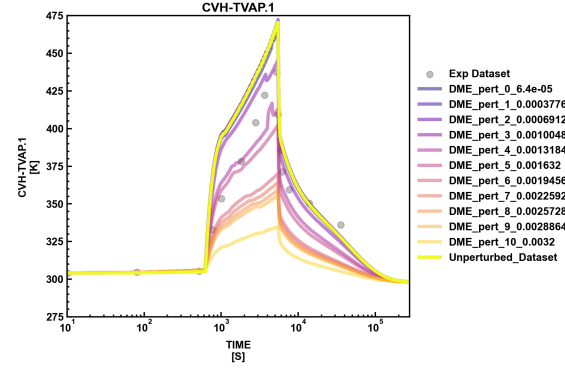
(r) Pool Mass, NaI

B.2. NAC_INPUT

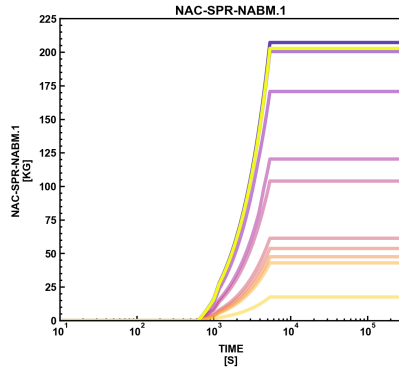
B.2.1. DME



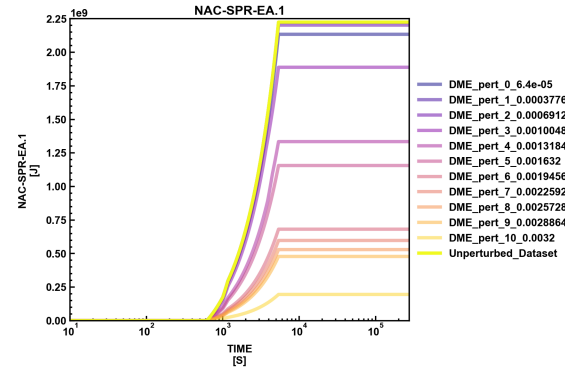
(a) Pressure



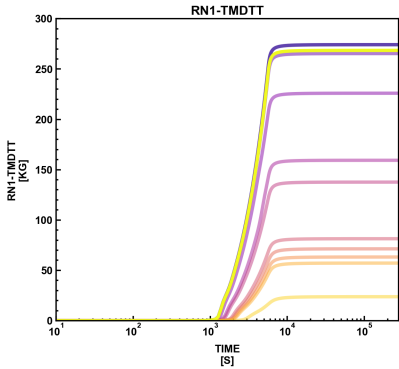
(b) Atmospheric Temperature



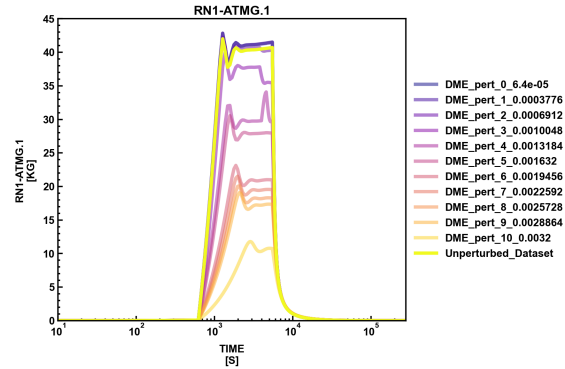
(c) Burned Sodium Mass



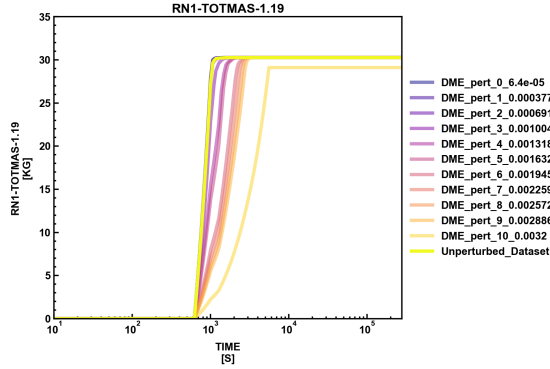
(d) Energy Input to Atmosphere



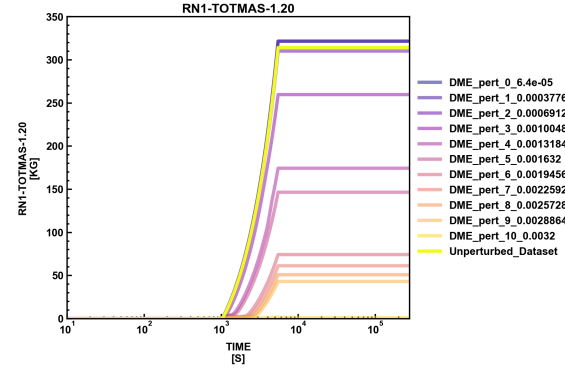
(e) Total Mass Deposited



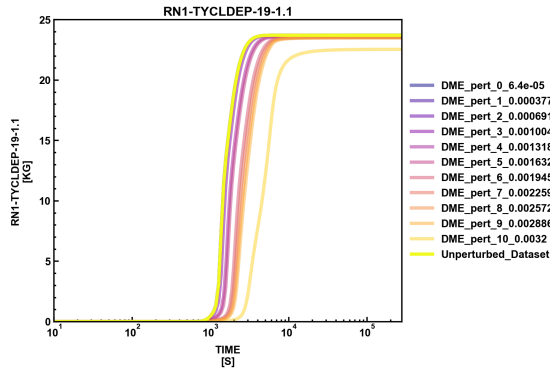
(f) Total Suspended Aerosol Mass



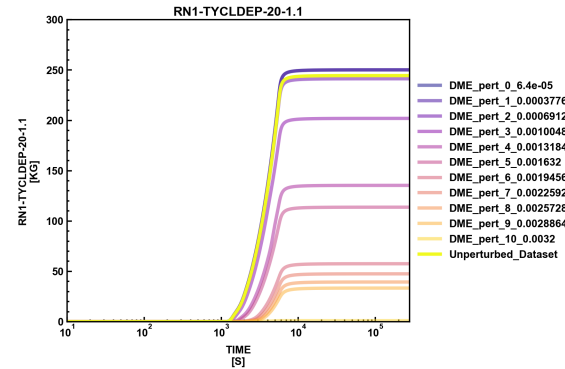
(g) Total Mass, NaOH



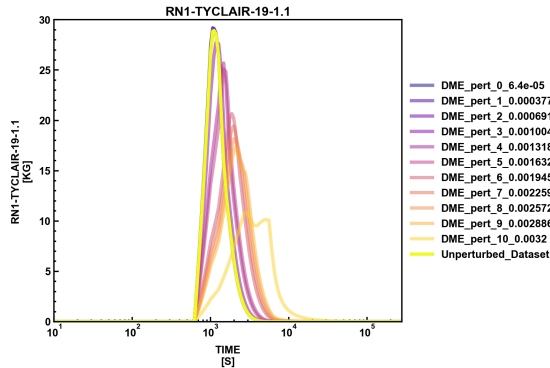
(h) Total Mass, Na₂O₂



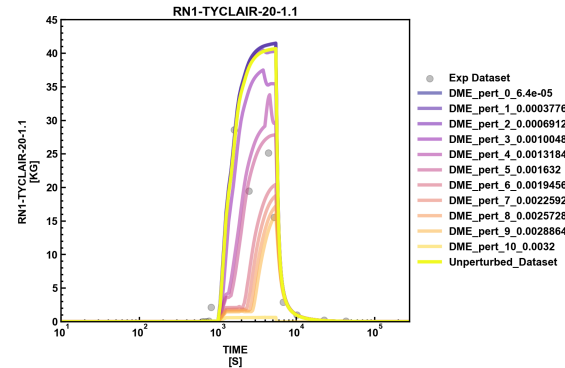
(i) Deposited Mass, NaOH



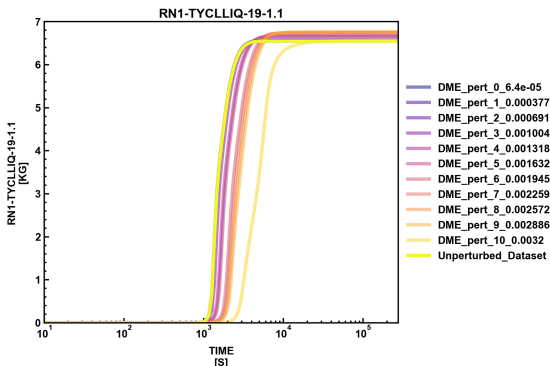
(j) Deposited Mass, Na₂O₂



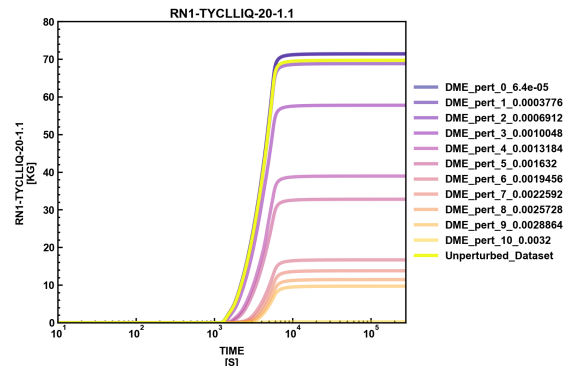
(k) Suspended Mass, NaOH



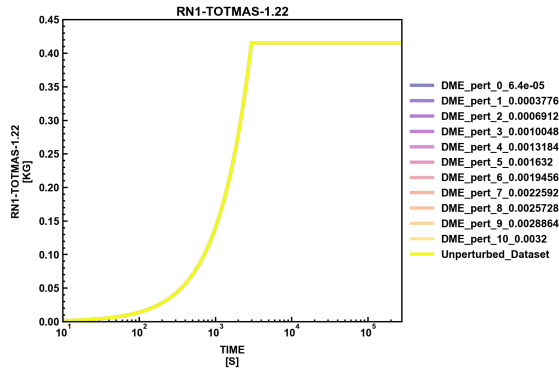
(l) Suspended Mass, Na₂O₂



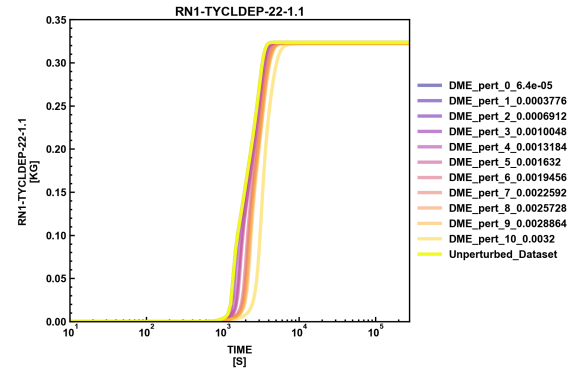
(m) Pool Mass, NaOH



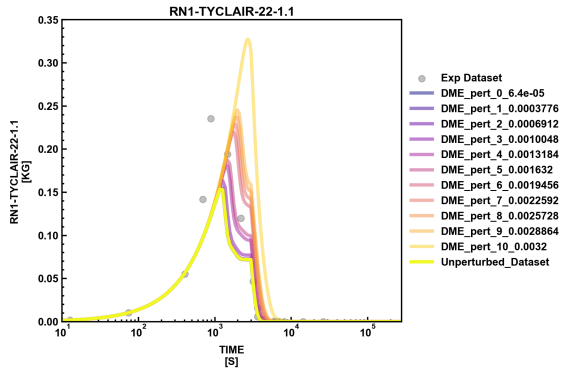
(n) Pool Mass, Na₂O₂



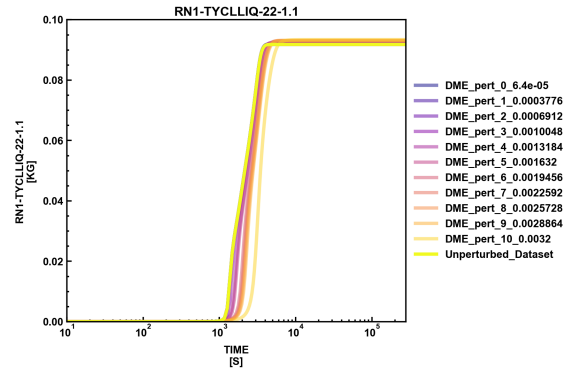
(o) Total Mass, NaI



(p) Deposited Mass, NaI

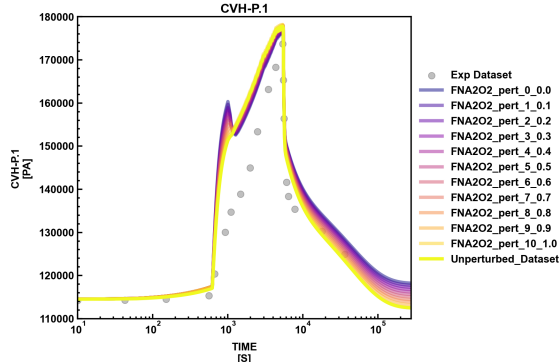


(q) Suspended Mass, NaI

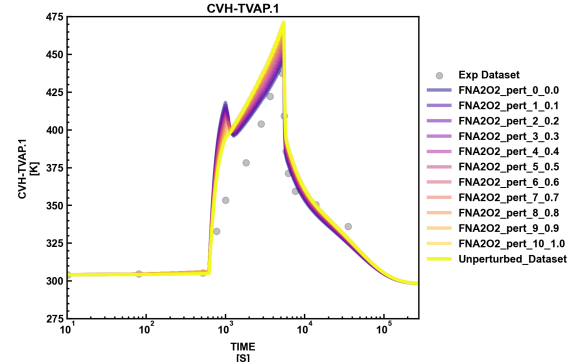


(r) Pool Mass, NaI

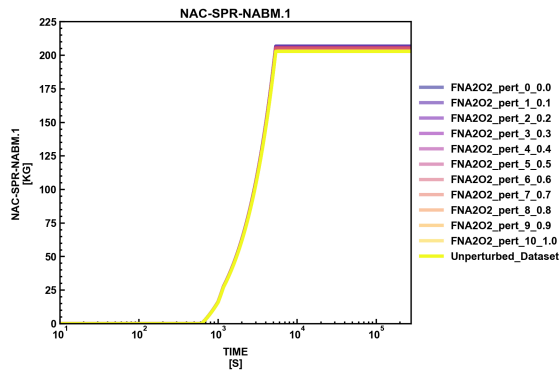
B.2.2. FNA202



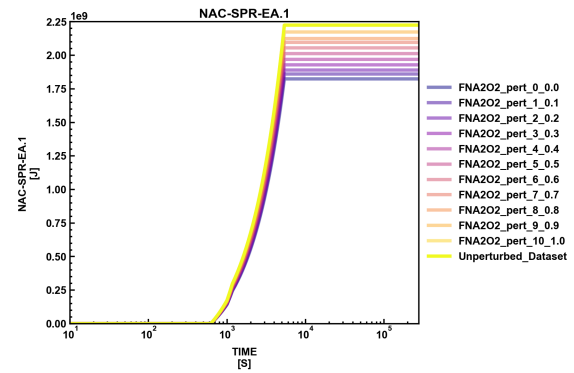
(a) Pressure



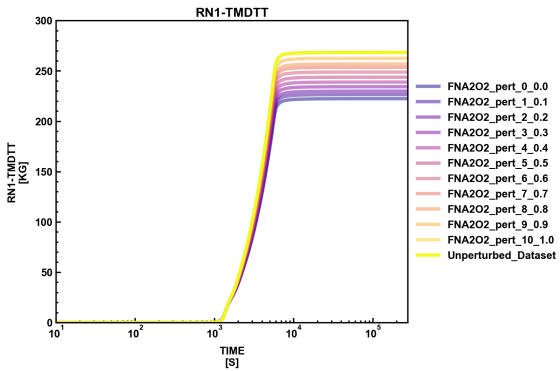
(b) Atmospheric Temperature



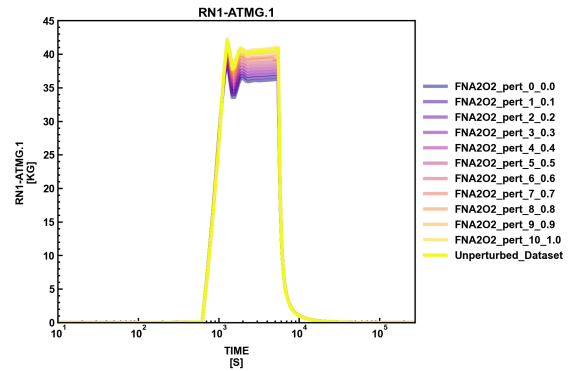
(c) Burned Sodium Mass



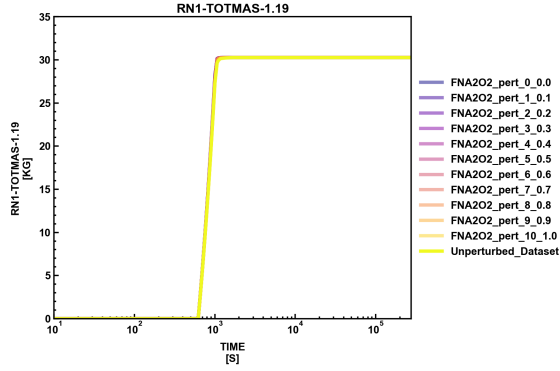
(d) Energy Input to Atmosphere



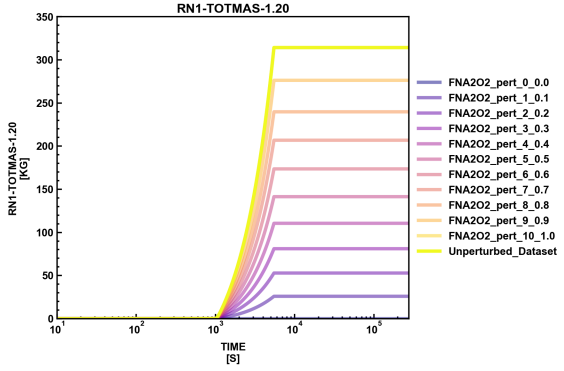
(e) Total Mass Deposited



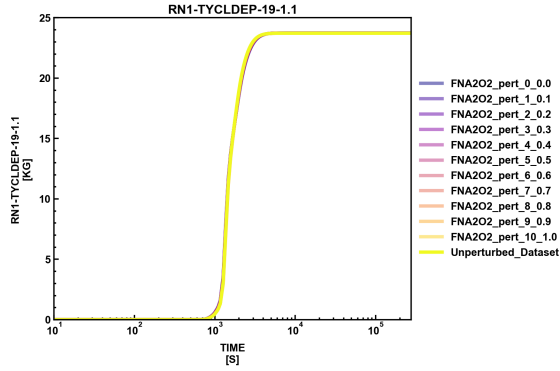
(f) Total Suspended Aerosol Mass



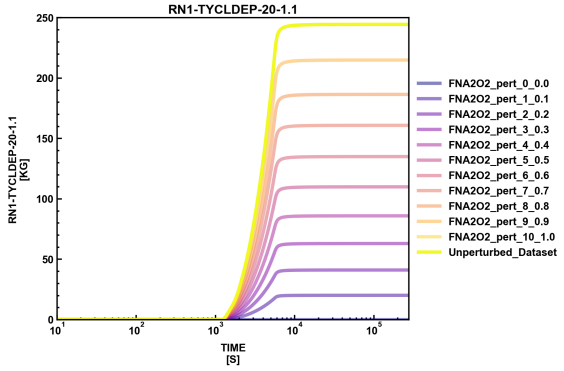
(g) Total Mass, NaOH



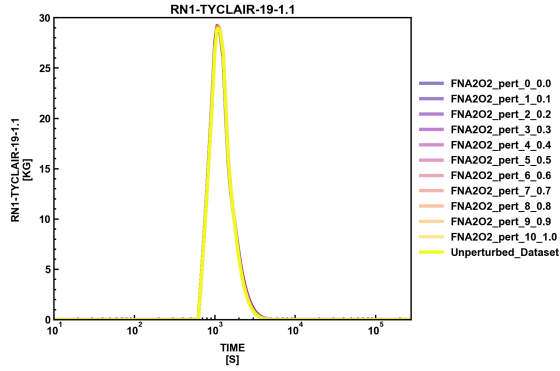
(h) Total Mass, Na₂O₂



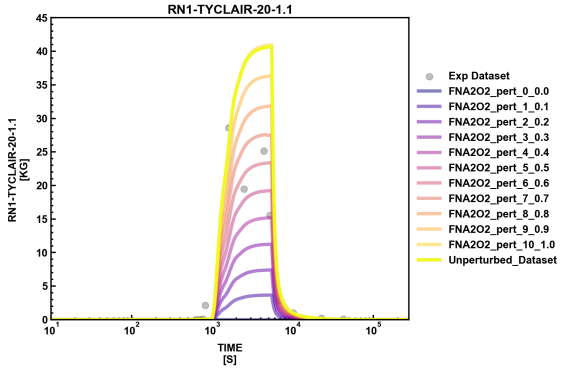
(i) Deposited Mass, NaOH



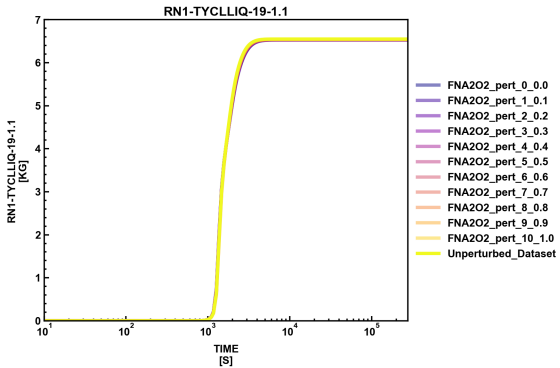
(j) Deposited Mass, Na₂O₂



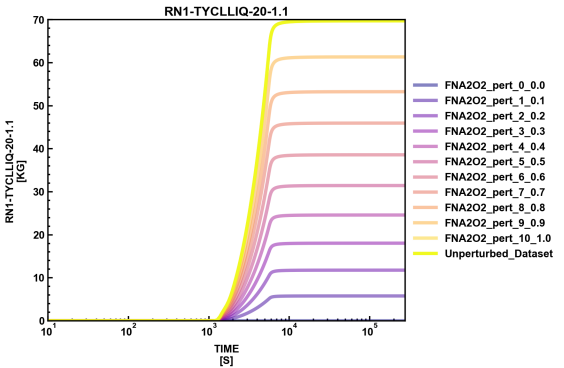
(k) Suspended Mass, NaOH



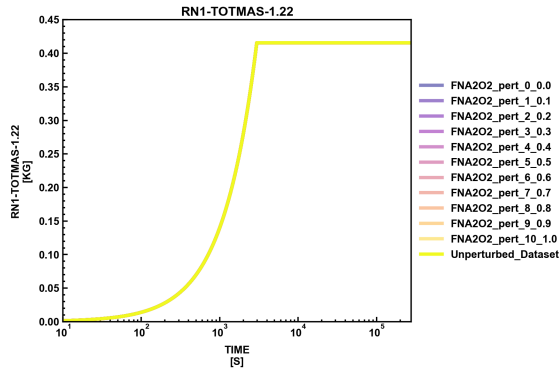
(l) Suspended Mass, Na₂O₂



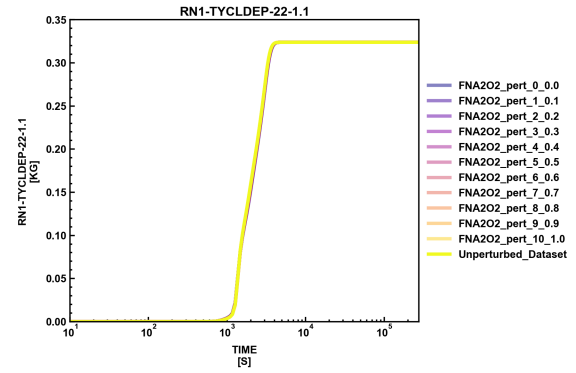
(m) Pool Mass, NaOH



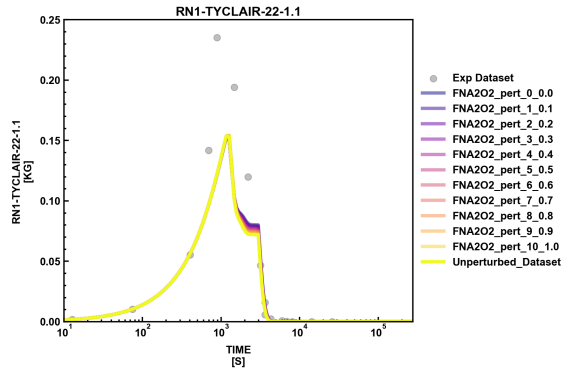
(n) Pool Mass, Na₂O₂



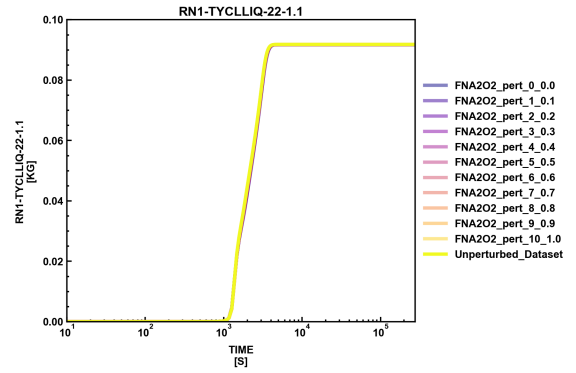
(o) Total Mass, NaI



(p) Deposited Mass, NaI

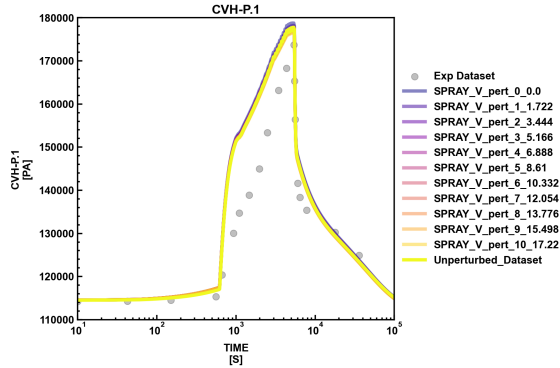


(q) Suspended Mass, NaI

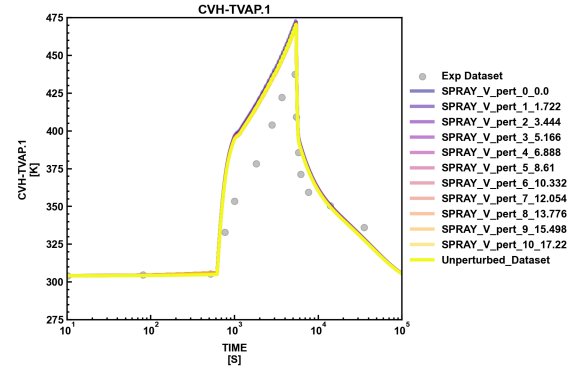


(r) Pool Mass, NaI

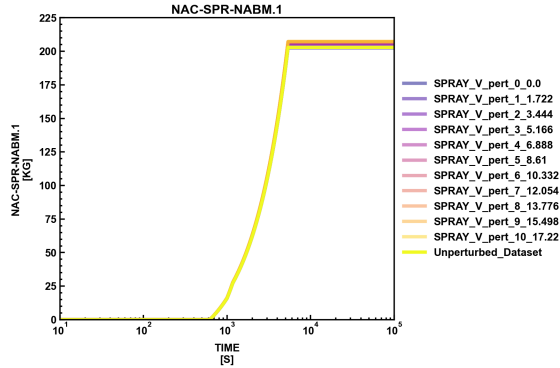
B.2.3. SPRAY_V



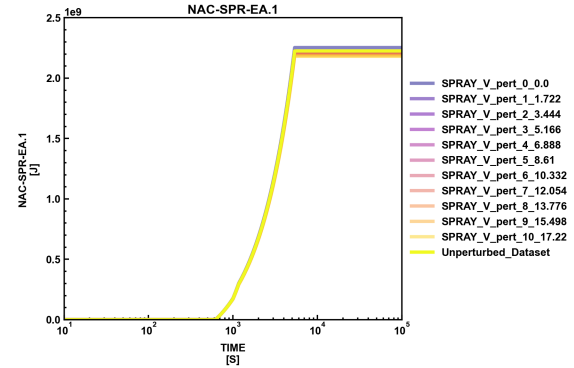
(a) Pressure



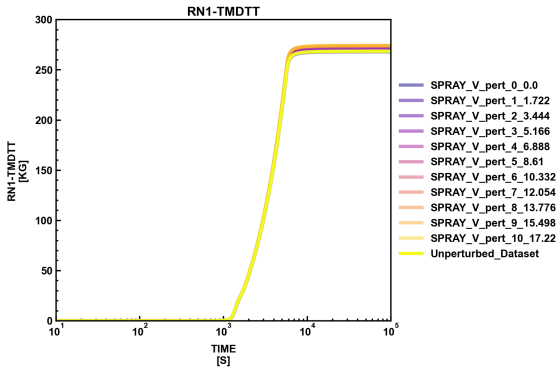
(b) Atmospheric Temperature



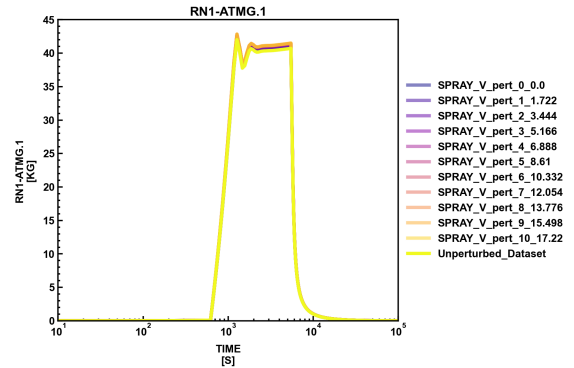
(c) Burned Sodium Mass



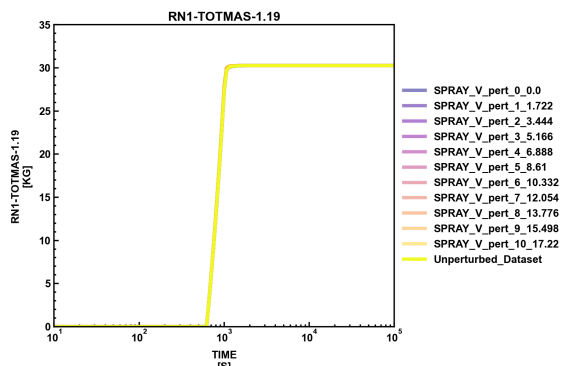
(d) Energy Input to Atmosphere



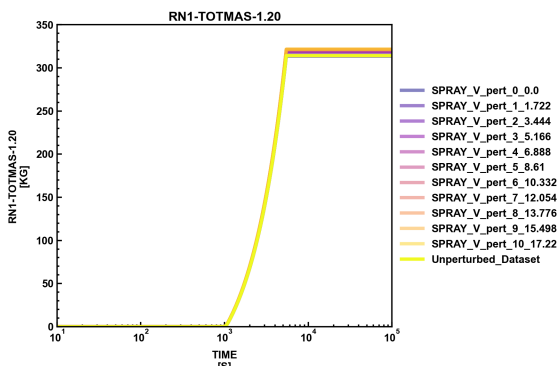
(e) Total Mass Deposited



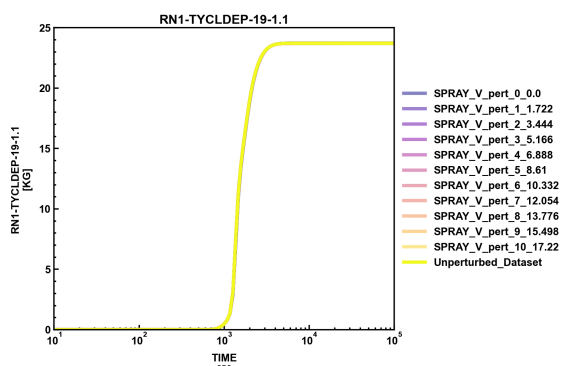
(f) Total Suspended Aerosol Mass



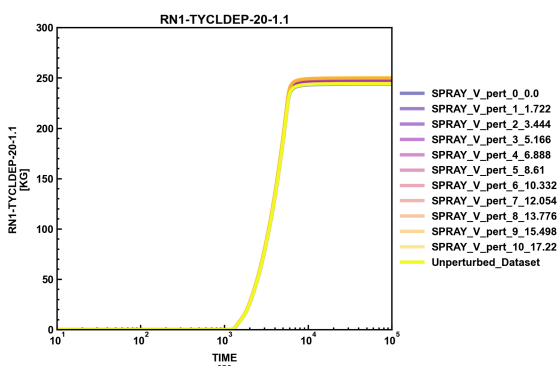
(g) Total Mass, NaOH



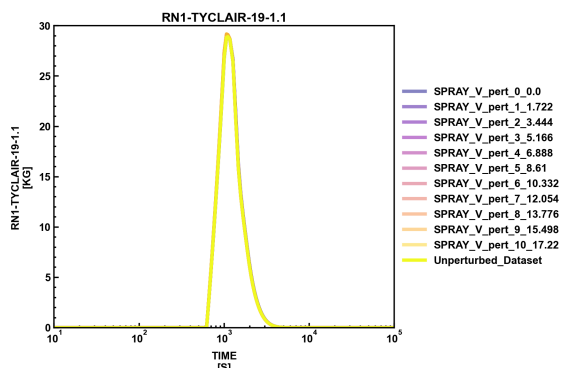
(h) Total Mass, Na₂O₂



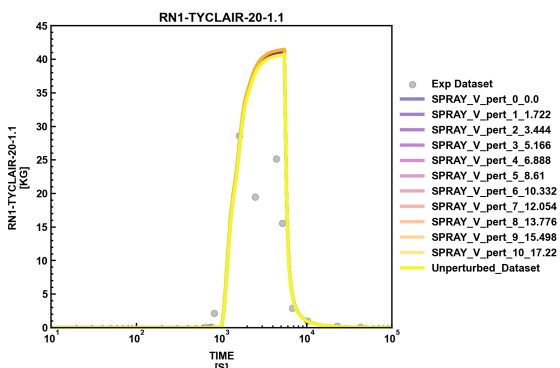
(i) Deposited Mass, NaOH



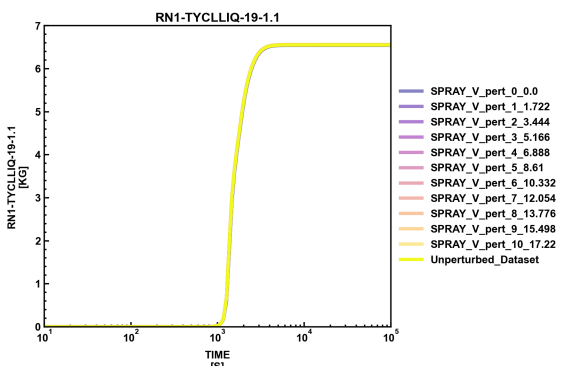
(j) Deposited Mass, Na₂O₂



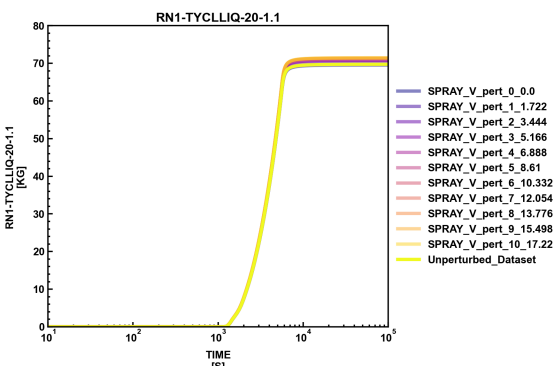
(k) Suspended Mass, NaOH



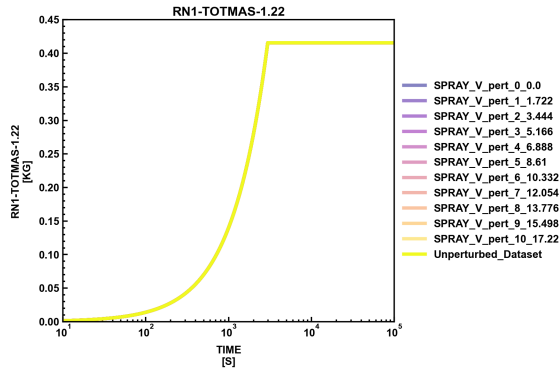
(l) Suspended Mass, Na₂O₂



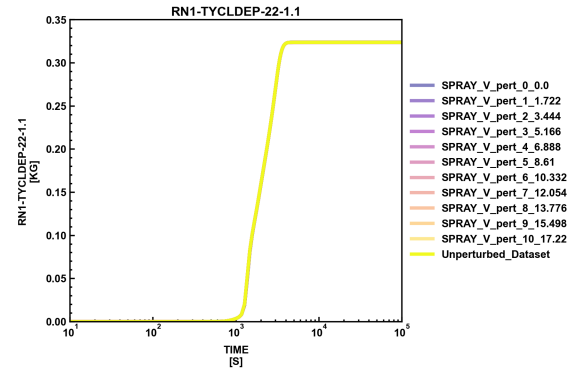
(m) Pool Mass, NaOH



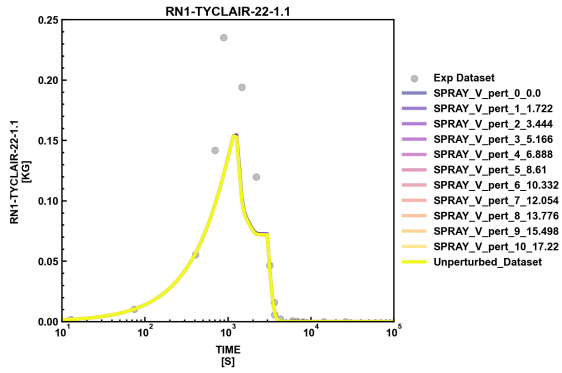
(n) Pool Mass, Na₂O₂



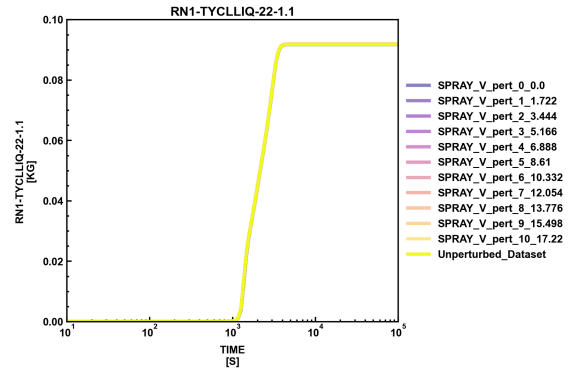
(o) Total Mass, NaI



(p) Deposited Mass, NaI



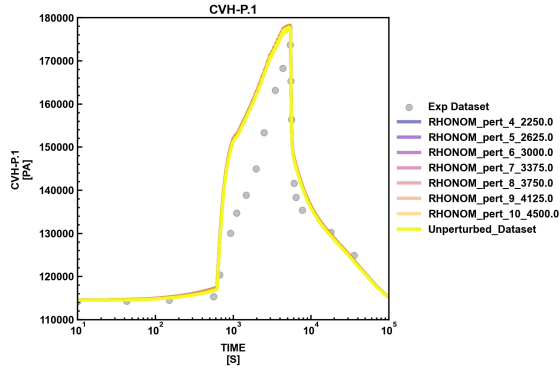
(q) Suspended Mass, NaI



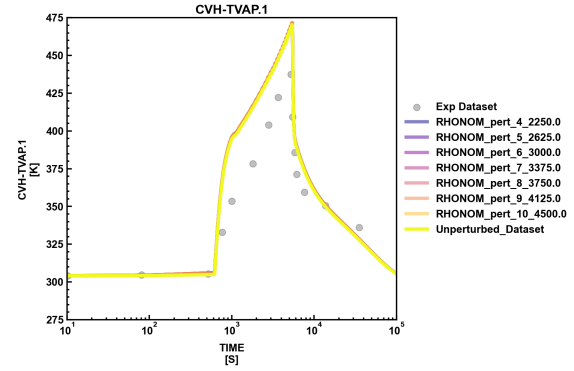
(r) Pool Mass, NaI

B.3. RN1_INPUT

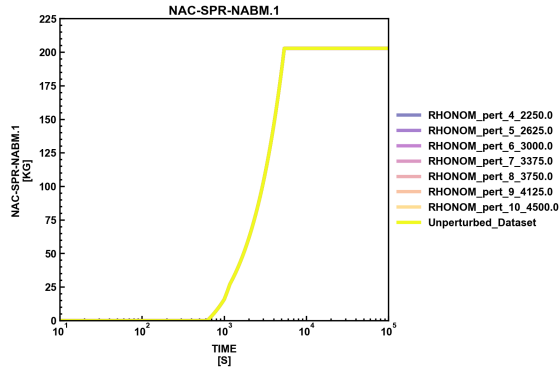
B.3.1. RHONOM



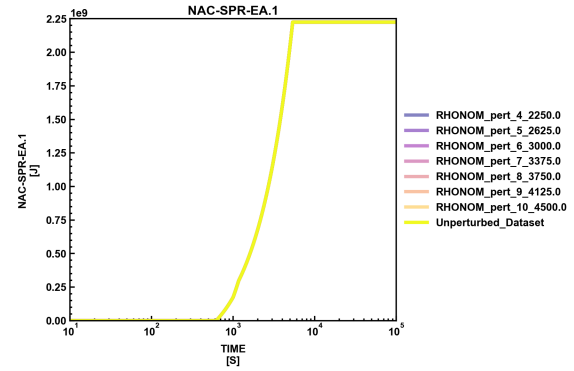
(a) Pressure



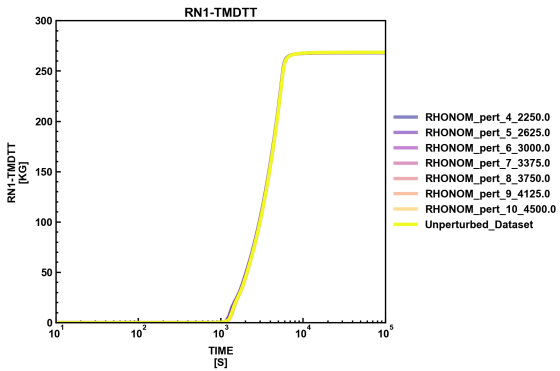
(b) Atmospheric Temperature



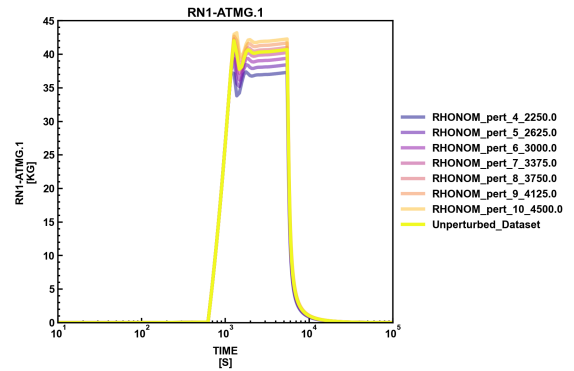
(c) Burned Sodium Mass



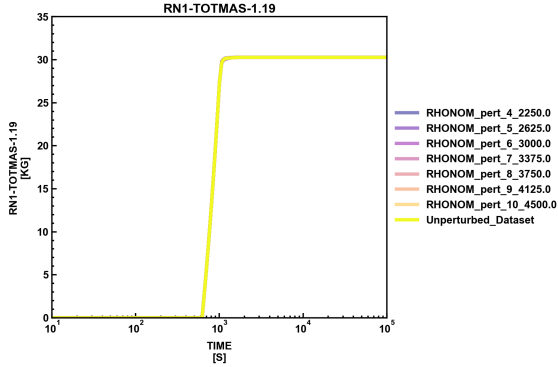
(d) Energy Input to Atmosphere



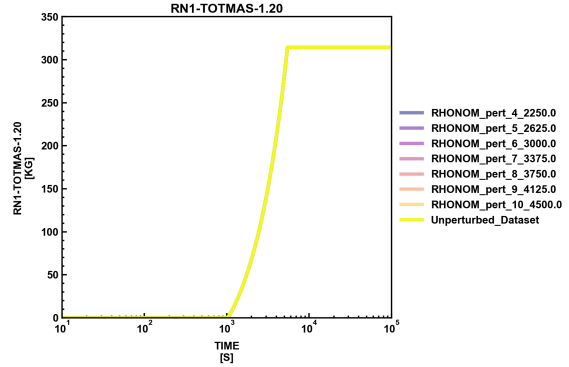
(e) Total Mass Deposited



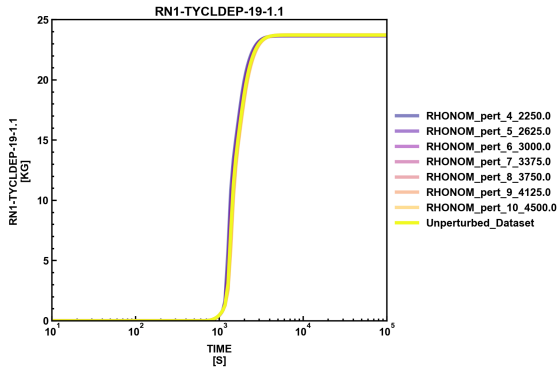
(f) Total Suspended Aerosol Mass



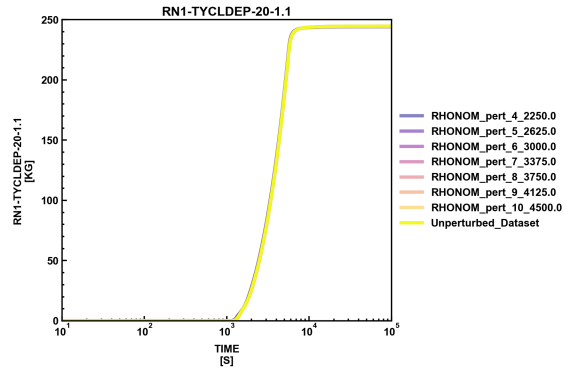
(g) Total Mass, NaOH



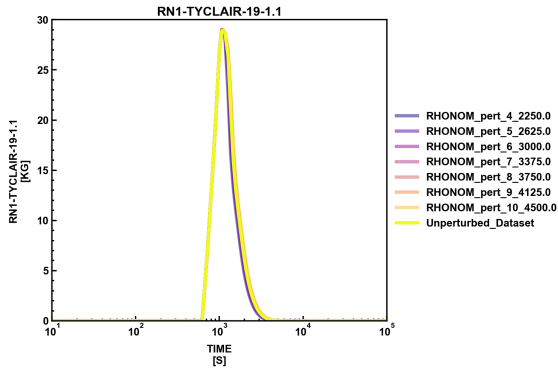
(h) Total Mass, Na₂O₂



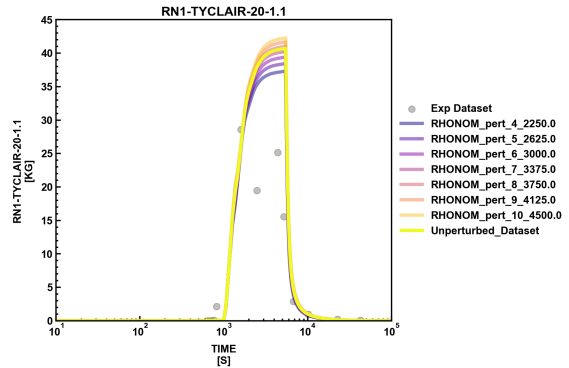
(i) Deposited Mass, NaOH



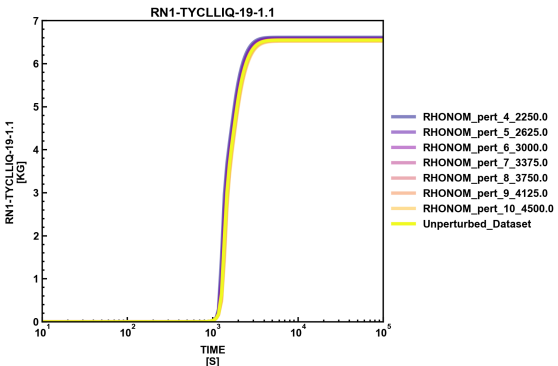
(j) Deposited Mass, Na₂O₂



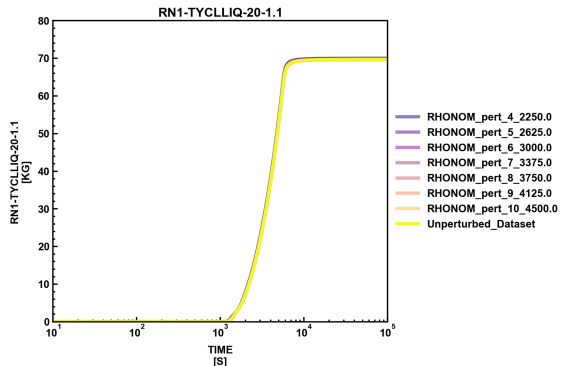
(k) Suspended Mass, NaOH



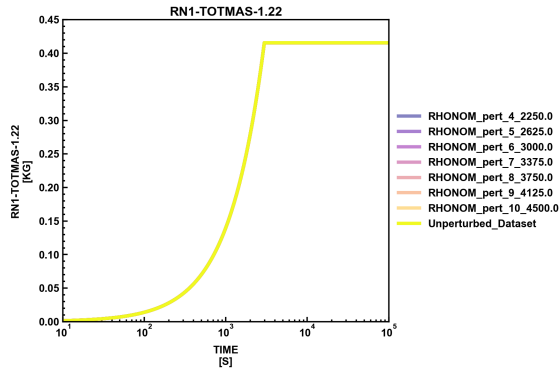
(l) Suspended Mass, Na₂O₂



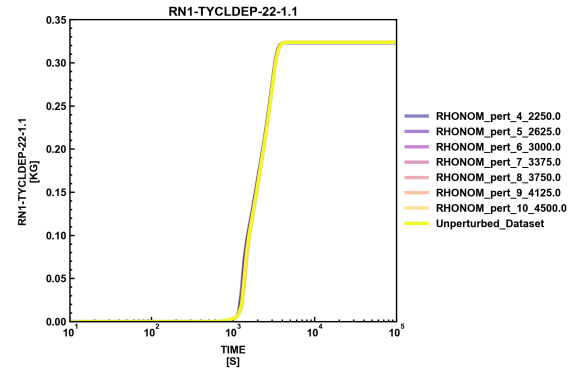
(m) Pool Mass, NaOH



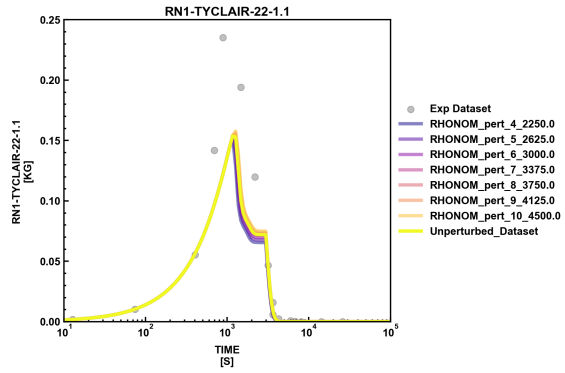
(n) Pool Mass, Na₂O₂



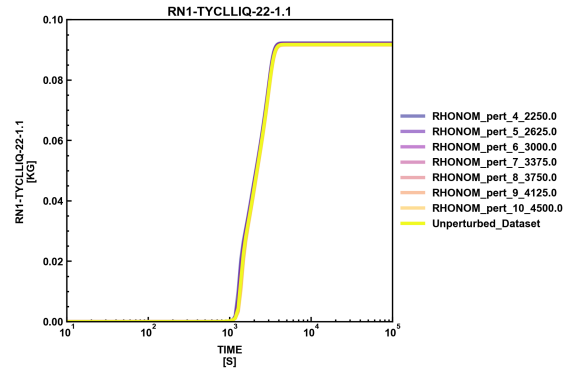
(o) Total Mass, NaI



(p) Deposited Mass, NaI

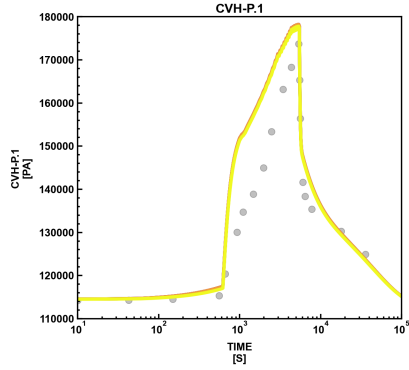


(q) Suspended Mass, NaI

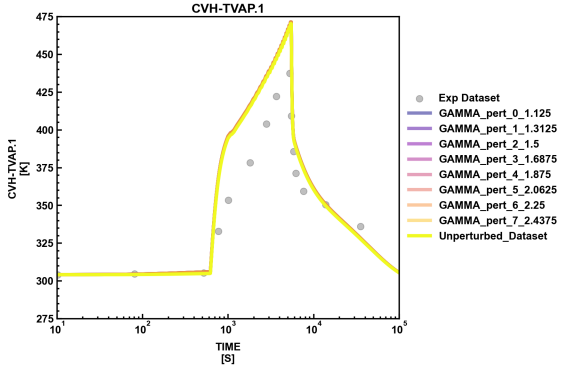


(r) Pool Mass, NaI

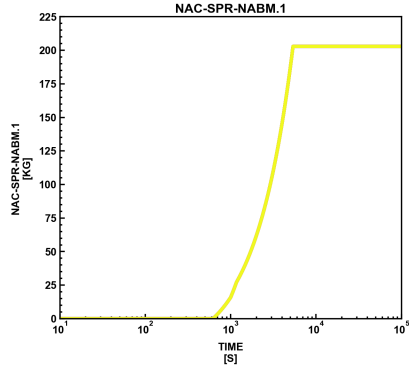
B.3.2. GAMMA



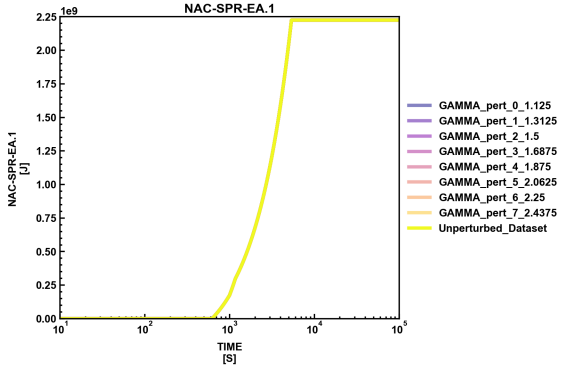
(a) Pressure



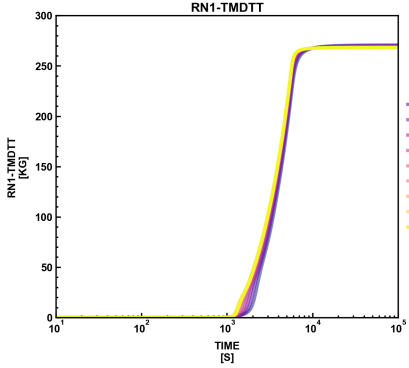
(b) Atmospheric Temperature



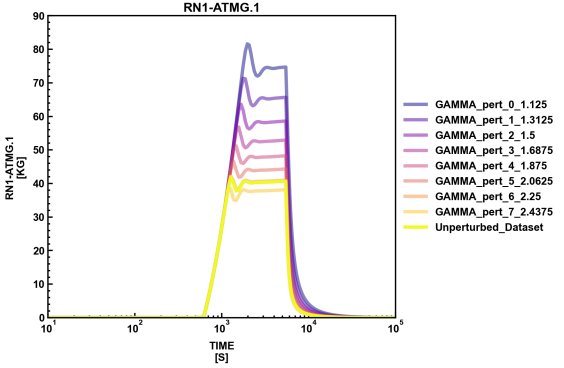
(c) Burned Sodium Mass



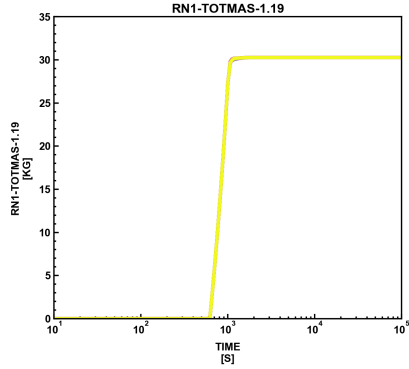
(d) Energy Input to Atmosphere



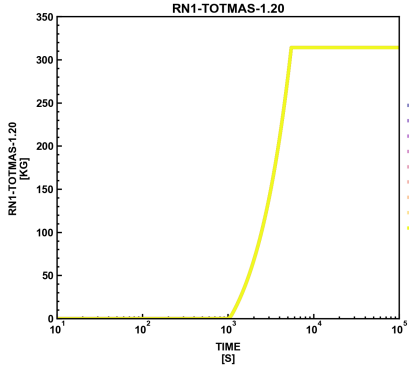
(e) Total Mass Deposited



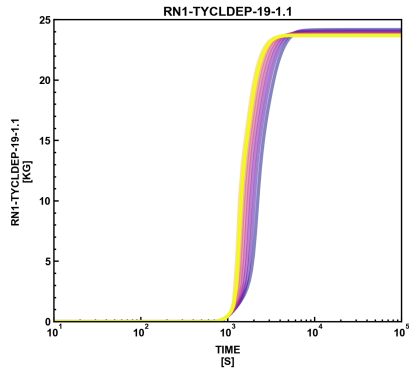
(f) Total Suspended Aerosol Mass



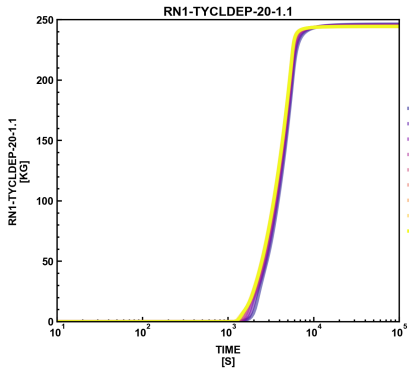
(g) Total Mass, NaOH



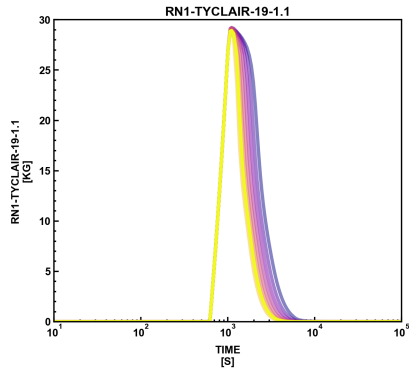
(h) Total Mass, Na₂O₂



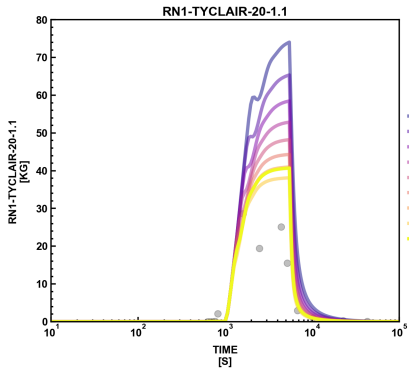
(i) Deposited Mass, NaOH



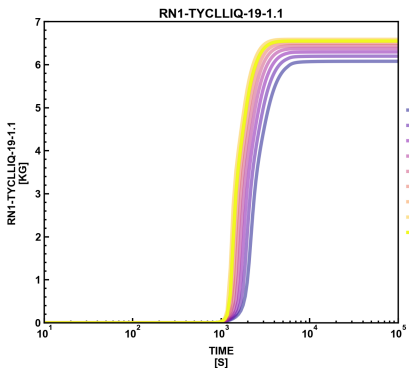
(j) Deposited Mass, Na₂O₂



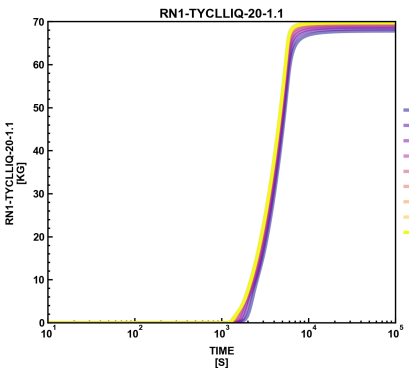
(k) Suspended Mass, NaOH



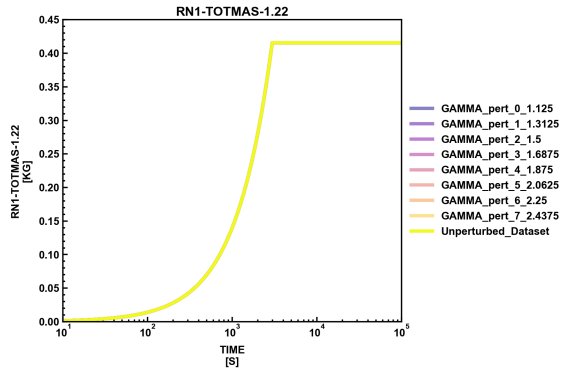
(l) Suspended Mass, Na₂O₂



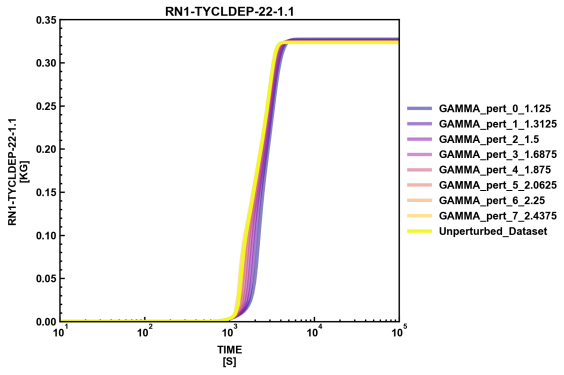
(m) Pool Mass, NaOH



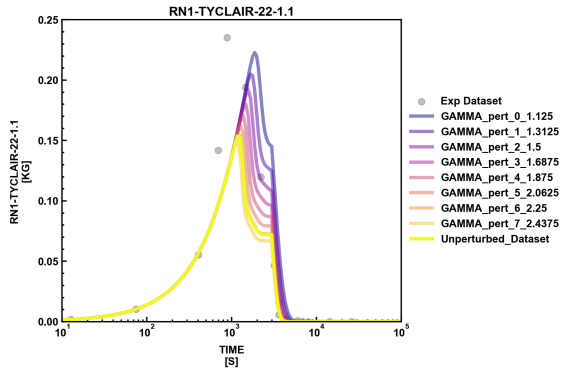
(n) Pool Mass, Na₂O₂



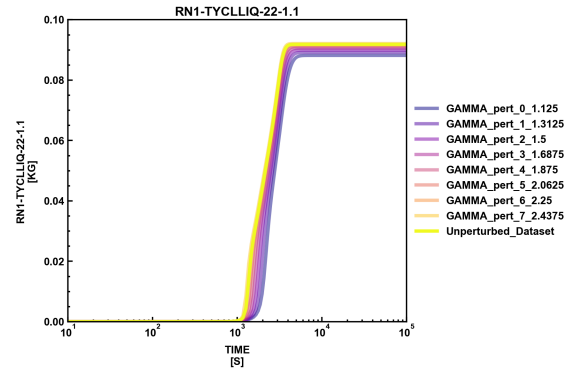
(o) Total Mass, NaI



(p) Deposited Mass, NaI

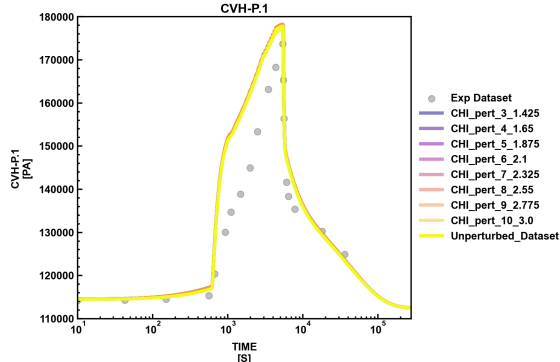


(q) Suspended Mass, NaI

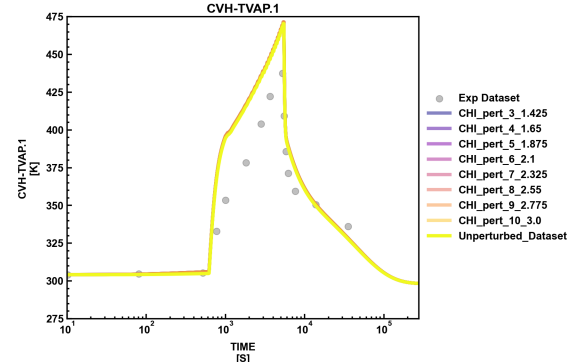


(r) Pool Mass, NaI

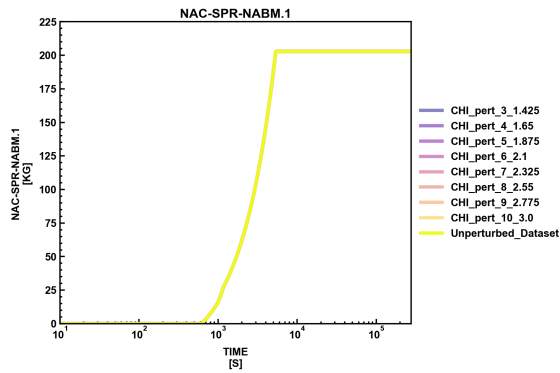
B.3.3. CHI



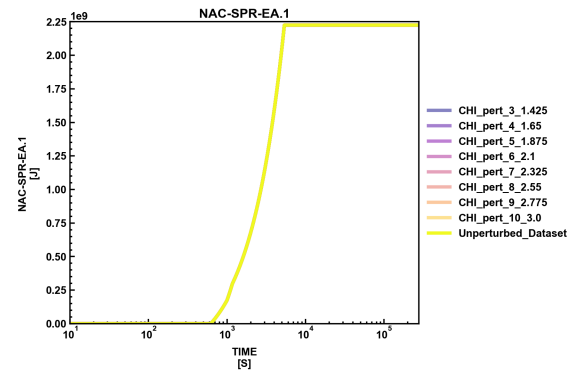
(a) Pressure



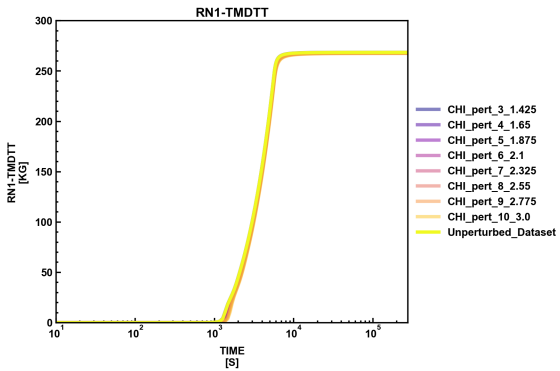
(b) Atmospheric Temperature



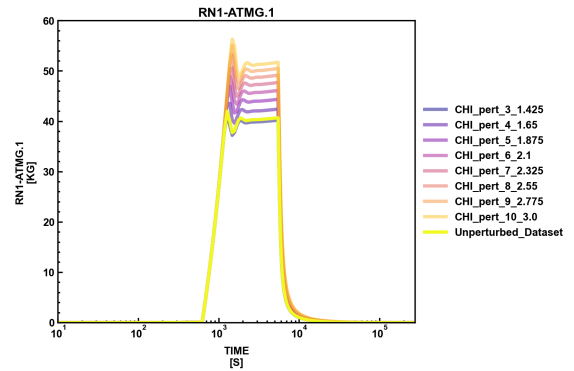
(c) Burned Sodium Mass



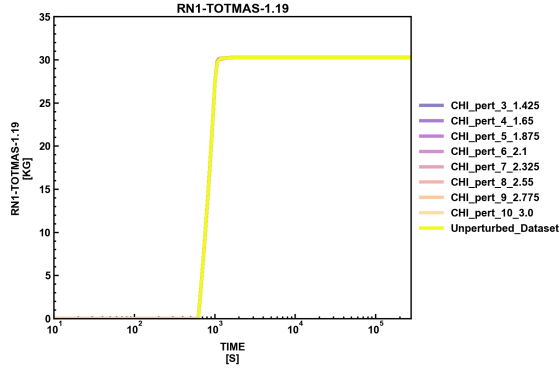
(d) Energy Input to Atmosphere



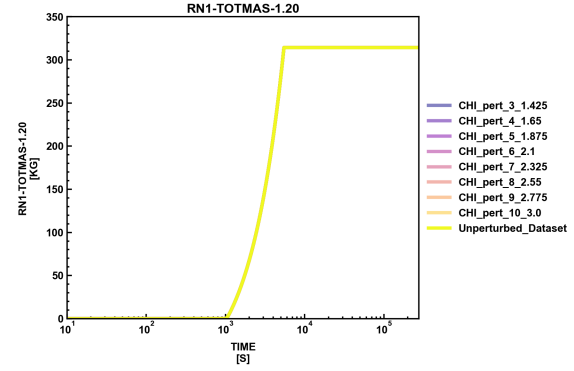
(e) Total Mass Deposited



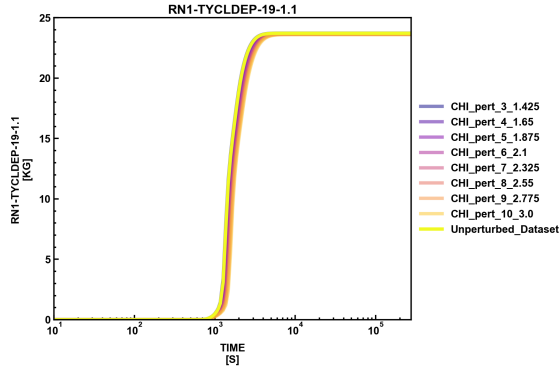
(f) Total Suspended Aerosol Mass



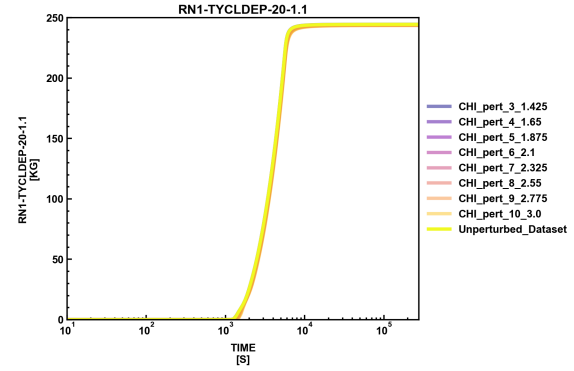
(g) Total Mass, NaOH



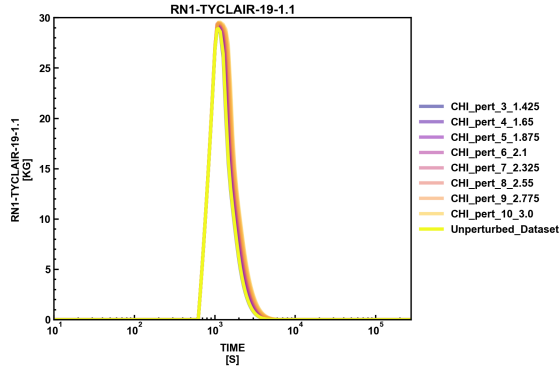
(h) Total Mass, Na_2O_2



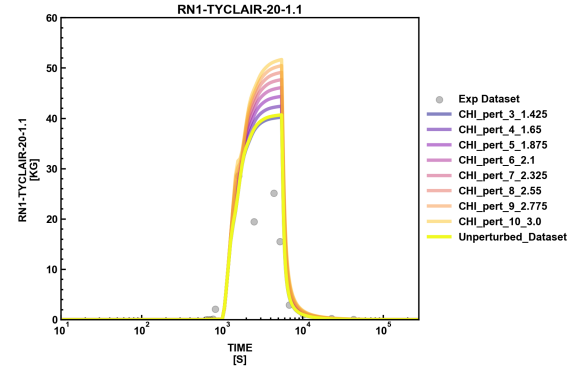
(i) Deposited Mass, NaOH



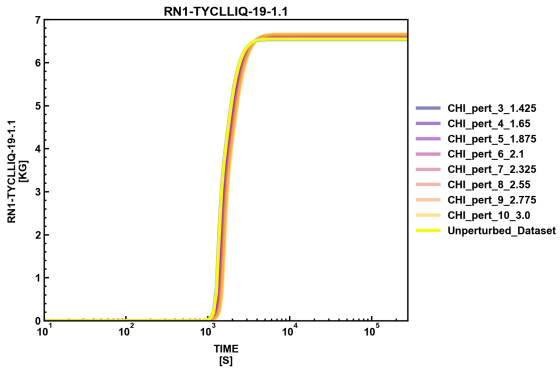
(j) Deposited Mass, Na_2O_2



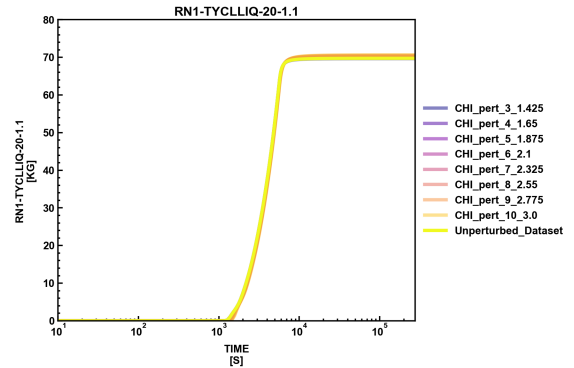
(k) Suspended Mass, NaOH



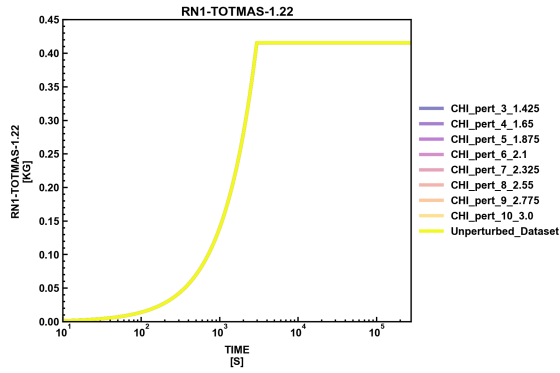
(l) Suspended Mass, Na_2O_2



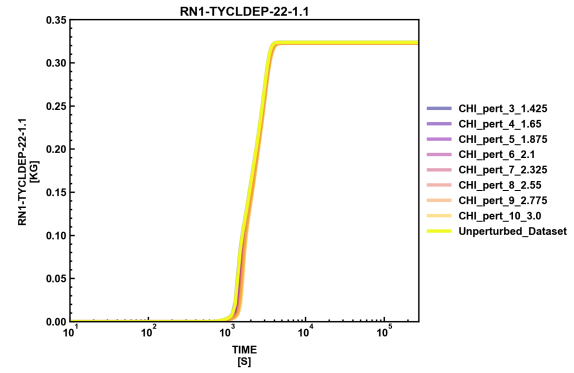
(m) Pool Mass, NaOH



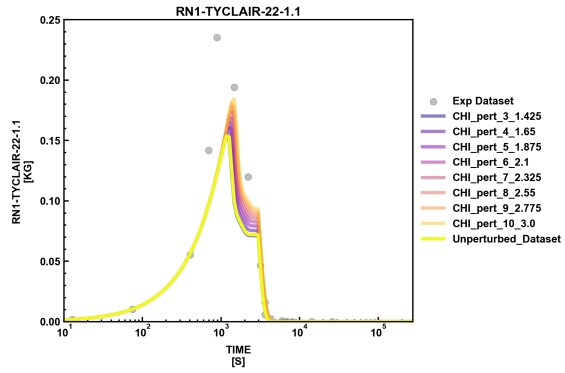
(n) Pool Mass, Na_2O_2



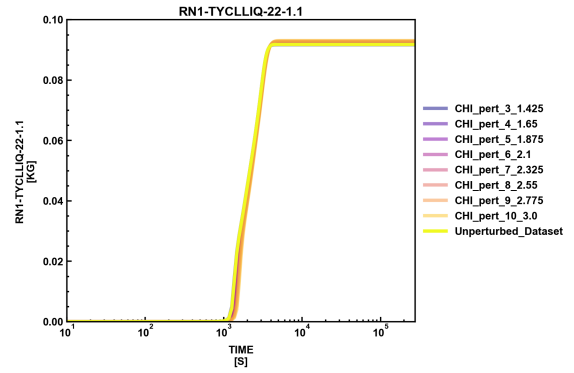
(o) Total Mass, NaI



(p) Deposited Mass, NaI



(q) Suspended Mass, NaI



(r) Pool Mass, NaI

C.1. AB5

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```

18 RN1-VDEP('top head',LHS,'NAOH',TOT)
19 RN1-VDEP('walls-edge',LHS,'NAOH',TOT)
20 RN1-VDEP('vert-int',LHS,'NAOH',TOT)
21 RN1-VDEP('floor',LHS,'NAOH',TOT)
22 RN1-VDEP('horiz-int',LHS,'NAOH',TOT)
!)

```

```

! #####
TF_INPUT ! (
! #####

```

```

!               tfname      tfscal      tfadcn
TF_ID           'EXHEAT'      1.0        0.0 ! (
!      size
TF_TAB      5 !n           x           y
              1           0.0           0.0
              2          12.9           0.0
              3          13.0          3.31E+05
              4          885.0          2.89E+09
              5          5.136E5          3.05E+09
!)

```

```

! #####
! TABULAR FUNCTION FOR AEROSOL SOURCE
! #####

```

```

!               tfname      tfscal      tfadcn
TF_ID           'ASOURCE'      1.0        0.0 ! (
!      size
TF_TAB      5 !n           x           y
              1           0.0           0.0
              2          12.95           0.0
              3          13.00           1.0
              4          885.00           1.0
              5          886.00           0.0
!)

```

```

!               tfname      tfscal      tfadcn
TF_ID           'CPS-F'        1.0        0.0 ! (
!      size
TF_TAB      2 !n           x           y
              1           0.0           0.0
              2           0.0          753.0
!)

```

```

!               tfname      tfscal      tfadcn
TF_ID           'THC-F'        1.0        0.0 ! (
!      size
TF_TAB      2 !n           x           y
              1           0.0           0.0
              2           0.0          0.0467
!)

```

```

!               tfname      tfscal      tfadcn
TF_ID           'RHO-F'        1.0        0.0 ! (
!      size
TF_TAB      2 !n           x           y
              1           0.0           0.0
              2           0.0          96.0
!)

```

```

! #####
! TABULAR FUNCTION FOR HEAT TRANSFER
! #####

```

```

!               tfname      tfscal      tfadcn
TF_ID           'CSTF-TEMP'      1.0        0.0 ! (
!      size
TF_TAB      2 !n           x           y
              1           0.0          298.15
              2          5.14E5          298.15
!

```

```

! sodium spray source and temperature
!

```

```

!               tfname      tfscal      tfadcn
TF_ID           'SPRAY-M'        1.0        0.0 ! (

```

```

!      size
TF_TAB  6 !n      x      y
      1      0.0      0.000
      2      12.9      0.000
      3      13.0      0.256
      4      885.0      0.256
      5      885.1      0.000
      6      10000.0      0.000

!
!      tfname      tfscal      tfadcn
TF_ID      'SPRAY-T'      1.0      0.0 !
!      size -- changed 5 to 6 steps to match -m and -s
TF_TAB  6 !n      x      y
      1      0.0      0.000
      2      12.9      0.000
      3      13.0      836.15
      4      885.0      836.15
      5      885.1      0.000
      6      10000.0      0.000

!
!      tfname      tfscal      tfadcn
TF_ID      'SPRAY-V'      1.0      0.0 !
!      size
TF_TAB  6 !n      x      y
      1      0.0      0.000
      2      12.9      0.000
      3      13.0      -5.216
      4      885.0      -5.216
      5      885.1      0.000
      6      10000.0      0.000

!
! model o2 injection rate, tstart=60s, tend=840s
! 47.6 m3 (STD), 0.02241 m3= 1mole-> 2123.67 moles of O2
! total injected 68 kgs. or 0.08718 kg/s
!
!      tfname      tfscal      tfadcn
TF_ID      'O2SOURCE'      1.0      0.0 !
!      size
TF_TAB  6 !n      x      y
      1      0.0      0.0
      2      59.9      0.0
      3      60.0      0.08718
      4      840.0      0.08718
      5      840.1      0.0
      6      10000.0      0.0

!
! o2 temperature at 293 K
!      tfname      tfscal      tfadcn
TF_ID      'O2TEMP'      1.0      0.0 !
!      size
TF_TAB  5 !n      x      y
      1      0.0      302.25 ! 293.0
      2      60.0      302.25 ! 293.0
      3      840.0      302.25 ! 293.0
      4      840.1      302.25 ! 293.0
      5      10000.0      302.25 ! 293.0

TF_ID 'Pressure' 1.0 ! ( x
TF_BND 'POINT' 'POINT'
TF_TAB 27 ! (
1 9.98626 127689.00
2 16.0354 138565.00
3 22.7292 147203.00
4 32.2171 155840.00
5 46.8204 164798.00
6 64.7208 173757.00
7 96.4575 181752.00
8 130.069 189430.00
9 167.012 191023.00

```

```

10 219.856 193256.00
11 268.394 197414.00
12 344.505 200930.00
13 400.027 205089.00
14 476.27 209248.00
15 785.231 212434.00
16 848.401 199617.00
17 871.449 189684.00
18 918.072 178149.00
19 1042.43 167573.00
20 1154.17 157958.00
21 1310.06 149304.00
22 2275.2 141596.00
23 4257.29 136769.00
24 7574.14 134186.00
25 13819.8 130321.00
26 23986.0 126137.00
27 44892.3 120028.00
!)
!)

!)
TF_ID 'Tvapor' 1.0 !( x
TF_BND 'POINT' 'POINT'
TF_TAB 16 !(
1 10.2153 301.345
2 21.7482 308.381
3 81.667 402.243
4 154.631 453.433
5 227.838 484.457
6 335.911 505.409
7 441.455 533.325
8 593.72 558.143
9 875.222 581.42
10 1032.35 503.954
11 1161.0 456.702
12 3050.15 397.124
13 5296.76 363.854
14 10781.3 356.166
15 31687.4 335.337
16 43689.2 328.391
!)
!)
TF_ID 'AEROSOL' 1.0 !( x
TF_BND 'POINT' 'POINT'
TF_TAB 23 !(
1 102.318 25.2633
2 147.623 36.4956
3 169.378 68.8929
4 194.338 54.5148
5 352.585 113.767
6 443.37 134.472
7 544.902 99.5234
8 786.181 102.908
9 1034.96 58.2855
10 1493.24 11.7075
11 1877.72 8.37986
12 3329.57 2.12716
13 5386.95 0.921999
14 14762.3 0.16752
15 18563.4 0.156683
16 21299.0 0.0917605
17 40454.3 0.0240848
18 62520.1 0.00944286
19 86163.5 0.00517241
20 108349.0 0.002397
21 163655.0 0.00114859
22 290193.0 0.000230712

```

23 428391.0 0.0001

!)

!)

! #####

CF_INPUT

! #####

CF_ID 'Pressure (exp)' 401 TAB-FUN ! (

CF_UNITS 'Pa'

CF_SAI 1.0 0.0 0.0 ! CFSCAL CFADCN CFVALR (INITIAL VALUE)

CF_MSC 'Pressure'

CF_ARG 1 ! NARG CHARG ARSCAL ARADCN

1 EXEC-TIME 1.0 0.0

!)

CF_ID 'T Vapor (exp)' 402 TAB-FUN ! (

CF_UNITS 'K'

CF_SAI 1.0 0.0 0.0 ! CFSCAL CFADCN CFVALR (INITIAL VALUE)

CF_MSC 'Tvapor'

CF_ARG 1 ! NARG CHARG ARSCAL ARADCN

1 EXEC-TIME 1.0 0.0

!)

CF_ID 'Aer Mass (exp)' 403 TAB-FUN ! (

CF_UNITS 'Kg'

CF_SAI 1.0 0.0 0.0 ! CFSCAL CFADCN CFVALR (INITIAL VALUE)

CF_MSC 'AEROSOL'

CF_ARG 1 ! NARG CHARG ARSCAL ARADCN

1 EXEC-TIME 1.0 0.0

!)

CF_ID 'Pressure' 501 EQUALS ! (

CF_UNITS 'Pa'

CF_SAI 1.0 0.0 0.0 ! CFSCAL CFADCN CFVALR (INITIAL VALUE)

CF_ARG 1 ! NARG CHARG ARSCAL ARADCN

1 CVH-P('CSTF') 1.0 0.0

!)

CF_ID 'T Vapor' 502 EQUALS ! (

CF_UNITS 'K'

CF_SAI 1.0 0.0 0.0 ! CFSCAL CFADCN CFVALR (INITIAL VALUE)

CF_ARG 1 ! NARG CHARG ARSCAL ARADCN

1 CVH-TVAP('CSTF') 1.0 0.0

!)

CF_ID 'Aer Mass' 503 EQUALS ! (

CF_UNITS 'Kg'

CF_SAI 1.0 0.0 0.0 ! CFSCAL CFADCN CFVALR (INITIAL VALUE)

CF_ARG 1 ! NARG CHARG ARSCAL ARADCN

1 RNI-ATMG('CSTF') 1.0 0.0

!)

!)

!)

! #####

MP_INPUT ! (

! #####

! matnam

MP_ID 'fiberglass' ! (

! size

MP_PRTF 3 !n prop itbprp cfkey

1 CPS 'CPS-F'

2 THC 'THC-F' TF

3 RHO 'RHO-F'

!)

! matnam

MP_ID CARBON-STEEL

!)

! #####

NCG_INPUT ! (

! #####

! mname

NCG_ID 'N2'

NCG_ID 'O2'

```

NCG_ID      'H2OV'
NCG_ID      'H2'
!)
! #####
DCH_INPUT !(
! #####
! NONE OF THESE ARE USED, THUS RCT, SHT, OPW, FPW ARE COMMENTED OUT
! EDIT: OPW IS NEEDED
!
!      reactp
DCH_RCT      PWR
!      shflg      tmshut
DCH_SHT      TIME      0.0
!      oprpow
DCH_OPW      0.0 ! 2.68597E9
!      u235p      pu239p      u238p
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 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'

!)
!)
! #####
CVH_INPUT !(
! #####
!
! CSTF - containment vessel
! Env - environment volume
!
!      cvname      icvnum

```

```

CV_ID          'CSTF'          1 ! (
!              icvtyp
CV_TYP          'CTYP-2'
!              icvthr          ipfsw          icvact
!CV_THR        EQUIL          FOG          ACTIVE
CV_THR          NONEQUIL          FOG          ACTIVE

!              itypth          ipora (changed ONLYATM TO POOLANDATM )          vapor
CV_PAS          SEPARATE          ONLYATM          SUPERHEATED
!CV_PAS          SEPARATE          POOLANDATM          SATURATED          SUPERHEATED
!              ptdit          pvol
CV_PTD          PVOL          1.22E5
!              atmtd          tatm
CV_AAD          TATM          302.25

!              nmmt          ncgid          tdew
CV_NCG          4          RHUM          0.0
!              n          namgas          mass
!              1          'N2'          0.7558 ! 0.75987 ! 0.740 !0.767
!              2          'O2'          0.2296 ! 0.22697 ! 0.233 !0.233
3          'H2Ov'          0.0146 ! 0.01316 ! 0.027
4          'H2'          0.0000

!              size
CV_VAT          4 !n          cvz          cvvol
!              1          0.0          0.0
!              2          1.9          50.0
!              3          18.4          752.0
!              4          20.3          852.0
!!! CV_VAT          8 !n          cvz          cvvol
!!!          1          0.0          0.0
!!!          2          1.9          50.0
!!!          3          3.4          152.0
!!!          4          7.3          252.0
!!!          5          10.0          400.0
!!!          6          14.9          650.0
!!!          7          18.4          800.0
!!!          8          20.3          852.0
!!!
!              size
! comment out EXHEAT, since the reaction energy would be added by NAC
! however, it needs to model the o2 injection
!
! IFELSE == ((( IF NONAC PRESENT, DO FIRST BLOCK ABOVE "|||" ELSE, DO STUFF BELOW "|||" )))
((NONAC
CV_SOU          5 !n          ctyp          interp          iessrc          srcname
!              1          AE          INTEGRAL          TF          'EXHEAT'          1.0
!              !n          ctyp          interp          iessrc          srcname          idmat          scaling_factor
!              2          mass          rate          tf          'O2SOURCE'          O2          1.0
!              3          te          rate          tf          'O2TEMP'          -1
4          mass          rate          tf          'SPRAY-M' POOL          1.0
5          te          rate          tf          'SPRAY-T'          1
|||
CV_SOU          2 !n          ctyp          interp          iessrc          idmat
1          mass          rate          tf          'O2SOURCE'          O2          1.0
2          te          rate          tf          'O2TEMP'          -1
)))

!)
!              cvname          icvnum
CV_ID          'ENV'          2 ! (
!              icvtyp
CV_TYP          'CTYP-6'
!              icvthr (EQUIL TO NONEQUIL)          ipfsw          icvact
CV_THR          EQUIL          FOG          time-indep
!              itypth          ipora (changed ONLYATM TO POOLANDATM )          vapor
CV_PAS          SEPARATE          ONLYATM          SUPERHEATED
!              ptdit          pvol

```

```

CV_PTD          PVOL          1.20E5
!              atmid          tatm
CV_AAD          TATM          298.15
!              nmmat          ncgid          rhum
CV_NCG          2            RHUM          0.0
!              n              namgas          mass
!              1              'N2'          0.79
!              2              'O2'          0.21
!              bndid          vpol
!CV_BND          VPOL          0.0
!              size
CV_VAT          2 !n          cvz          cvvol
!              1              0.0          0.0
!              2              20.3         852.0
!)
!)
! #####
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'          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 = CSTF CYLINDER WALLS
!
!              hsname          ishnum
HS_ID          'walls-edge'          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'          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      395.0          7.62            16.5 !3.8
!           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'      3 !( 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'          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            7.62
!           ibcr           ibvr           mteval
HS_RB      CalcCoefHS      'CSTF'          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            7.62
!           iftnum
HS_FT      OFF
!)
! HS 4 = BOTTOM HEAD

```

```

!
!      hsname      ishnum
HS_ID      'floor'      4 !( 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'      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      7.62
!      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'      5 !( 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'      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'      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
!)
!)
! #####
RN1_INPUT 0 ! (
! #####
! dft
! RN1_DFT 1.86 ! comment out because EXEC Default flag is enabled for 2.0
!
! 20 = Number of sections, 2 = Number of aerosol components
! 1 = Number of tabular aerosol sources
! Note that number of sections used was chosen based on the original deck developed
! It is not expected that significant difference in results if default number sections used (10)
!
! //// Need to add na2o2, na2o for aerosols
!
!
!
! numsec numcmp numcls numca
!!! ((10sect
!!! RN1_DIM 10 3 21 6
!!! |||
!!! RN1_DIM 20 3 21 6
!!! )))
!!!
! numsec numcmp numcls numca
RN1_DIM 20 3 21 6
! iclnrm
RN1_DCHNORM NONE
! dmin dmax rhonom
! replaced dmax 1.0E-5 with 5.0E-5 (DME value from NAC) default value is 5.0E-5
! replaced rhonom 2500 with 500 (DME value from NAC)
!!! RN1_ASP 1.0E-8 5.0E-5 817.0
! Best applies to when Na fire is turned off?
RN1_ASP 1.0E-8 5.0E-5 2500.0
! icoeff (changed CALANDWR to CALCUL)
RN1_ACOEF CALCUL
! pgas1 pgas2 tgas1 tgas2 (changed upper limit from 700 to 800)
RN1_PT 50000.0 6.0E6 270.0 1000.0
! DEFAULT AEROSOL VALUES
! (
! 1.0 = Dynamic shape factor
! 1.0 = Agglomeration shape factor
! 1.257 = Slip coefficient
! 1.0 = Sticking coefficient
! 0.001 = Turbulence dissipation
! 0.05 = gas thermal cond./part. th. cond.
! 2.25 = thermal accomodation coefficient
! 1.0e-5 = Diffusion boundary layer thickness
!
! THESE GUYS HAVE THE STRONGEST EFFECTS ON PLATED MASSES
! chi gamma fslip stick
!RN1_MS00 1.5 2.25 1.37 0.5
RN1_MS00 1.5 2.25 1.37 1.0
! Best applies to when Na fire is turned off?
!!! RN1_MS00 1.5 2.25 1.37 0.5
! turbds tkgop ftherm deldif
! tkgop (changed 0.05 to 0.00019 = 0.02662/140 W/m K) ---> consider void space in aerosol...
!RN1_MS01 2.5E-3 0.05 2.25 1.0E-5
RN1_MS01 1.0E-3 0.05 1.00 1.0E-5

! !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!)
! size
RN1_DS 7 !n ids isde ityp
1 'top head' LHS CEILING
2 'walls-edge' LHS WALL
3 'vert-int' LHS WALL

```

```

4      'floor'          LHS      FLOOR
5      'horiz-int'      LHS      FLOOR
6      'vert-int'       RHS      INACTIVE
7      'horiz-int'       RHS      INACTIVE
!      size
RN1_SET 1 !n          ivolf      ivolt      elev      area
          1          'ENV'      'ENV'      0.0      1.0
!      name      ivol      iphs      iclss      rfrs      xm      itab      cfnam
!RN1_AS 'AS000' 'CSTF' VAPOR 'NA' 0.0 0.445 TF 'ASOURCE'
!      idist      geommm      gsd
RN1_AS01 LOGNORMAL      5.0E-7      1.5
!      class      aerosol
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
!
! all new classes are required to input C7120, C7170
! 7130, 7136, 7141, 7102, 7111, 7120, 7131, 7132, 7170
! 7101, 7110
RN1_CSC 25 ! 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/
         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)

```



```

! Base input includes specification of all plant systems and severe accident
! physics.
!=====

!block: 'melgenbase'

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!      EXEC DATA      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

EXEC_INPUT ! (
EXEC_TITLE 'Sensitivity test AB6'
EXEC_DTIME 1.0E-3
EXEC_GLOBAL_DFT 2.0 ! global flag for 2.0 is used.
EXEC_JOBID 'REF'
EXEC_PLOT 34 ! (
1  RN1-TYCLAIR(NA2O2,'CTYP-2','TOT')
2  RN1-TYCLAIR(NAI,'CTYP-2','TOT')
3  RN1-ADEP('top head',LHS,'NA2O2',TOT)
4  RN1-ADEP('walls-edge',LHS,'NA2O2',TOT)
5  RN1-ADEP('vert-int',LHS,'NA2O2',TOT)
6  RN1-ADEP('floor',LHS,'NA2O2',TOT)
7  RN1-ADEP('horiz-int',LHS,'NA2O2',TOT)
8  RN1-ADEP('top head',LHS,'NAI',TOT)
9  RN1-ADEP('walls-edge',LHS,'NAI',TOT)
10 RN1-ADEP('vert-int',LHS,'NAI',TOT)
11 RN1-ADEP('floor',LHS,'NAI',TOT)
12 RN1-ADEP('horiz-int',LHS,'NAI',TOT)
13 RN1-VDEP('top head',LHS,'NAI',TOT)
14 RN1-VDEP('walls-edge',LHS,'NAI',TOT)
15 RN1-VDEP('vert-int',LHS,'NAI',TOT)
16 RN1-VDEP('floor',LHS,'NAI',TOT)
17 RN1-VDEP('horiz-int',LHS,'NAI',TOT)
18 RN1-VDEP('top head',LHS,'NA2O2',TOT)
19 RN1-VDEP('walls-edge',LHS,'NA2O2',TOT)
20 RN1-VDEP('vert-int',LHS,'NA2O2',TOT)
21 RN1-VDEP('floor',LHS,'NA2O2',TOT)
22 RN1-VDEP('horiz-int',LHS,'NA2O2',TOT)
23 RN1-TYCLAIR(CS,'CTYP-2','TOT')
24 RN1-ADEP('top head',LHS,'NAOH',TOT)
25 RN1-ADEP('walls-edge',LHS,'NAOH',TOT)
26 RN1-ADEP('vert-int',LHS,'NAOH',TOT)
27 RN1-ADEP('floor',LHS,'NAOH',TOT)
28 RN1-VDEP('horiz-int',LHS,'NAOH',TOT)
29 RN1-VDEP('top head',LHS,'NAOH',TOT)
30 RN1-VDEP('walls-edge',LHS,'NAOH',TOT)
31 RN1-VDEP('vert-int',LHS,'NAOH',TOT)
32 RN1-VDEP('floor',LHS,'NAOH',TOT)
33 RN1-ADEP('horiz-int',LHS,'NAOH',TOT)
34 RN1-TYCLAIR(NAOH,'CTYP-2','TOT')
!)
!)
#####
!
!  _____
!  | _ _ | _ | | _ \ _ _ | | _ _ _ _ _
!  | | | _ | | _ / _ / _ / / _ / _ / _
!  | _ | _ | | _ \ _ \ _ \ _ \ _ \ _
!
!  |____/
#####

TF_INPUT ! (
TF_ID      'EXHEAT'      1.0      0.0 ! (
TF_TAB      5 !n      x      y
      1      0.0      0.0
      2      619.9      0.0
      3      620.0      29400.0
      4      5400.0      2.86E9

```

```

5          2.77E5          3.0E9
!)
TF_ID      'O2SOURCE'          1.0          0.0 ! (
TF_TAB     6 !n          x          y
1          0.0          0.0
2          59.9          0.0
3          60.0          0.02073
4          4400.0          0.02073
5          4401.0          0.0
6          2.77E5          0.0
TF_ID      'O2TEMP'          1.0          0.0 ! (
TF_TAB     6 !n          x          y
1          0.0          0.0
2          59.9          0.0
3          60.0          302.0
4          4400.0          302.0
5          4401.0          0.0
6          2.77E5          0.0

! N2 source feeding in with NaI
TF_ID      'N2SOURCE'          1.0          0.0 ! (
TF_TAB     4 !n          x          y
1          0.0          0.017659
2          3000.0          0.017659
3          3001.0          0.0
4          2.77E5          0.0
TF_ID      'N2TEMP'          1.0          0.0 ! (
TF_TAB     4 !n          x          y
1          0.0          483.0
2          3000.0          483.0
3          3001.0          0.0
4          2.77E5          0.0
TF_ID      'ASOURCE2'          1.0          0.0 ! (
TF_TAB     4 !n          x          y
1          0.0          1.0
2          3000.0          1.0
3          3001.0          0.0
4          2.77E5          0.0
TF_ID      'SPRAY-M'          1.0          0.0 ! (
TF_TAB     6 !n          x          y
1          0.0          0.0
2          619.95          0.0
3          620.0          0.0428
4          5400.0          0.0428
5          5401.0          0.0
6          2.77E5          0.0
TF_ID      'SPRAY-T'          1.0          0.0 ! (
TF_TAB     6 !n          x          y
1          0.0          0.0
2          619.95          0.0
3          620.0          833.15
4          5400.0          833.15
5          5401.0          0.0
6          2.77E5          0.0
TF_ID      'SPRAY-V'          1.0          0.0 ! (
TF_TAB     6 !n          x          y
1          0.0          0.0
2          619.95          0.0
3          620.0          -1.722
4          5400.0          -1.722
5          5401.0          0.0
6          2.77E5          0.0
!)
TF_ID      'DECAY'          1.0          0.0 ! (
TF_TAB     2 !n          x          y
1          0.0          0.0
2          2.77E5          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      5.14E5    298.15
!)
!)
TF_ID 'Pressure'      1.0 ! ( x
TF_BND 'POINT' 'POINT'
TF_TAB  20 ! (
1 10.0 114212.0
2 42.6827 114326.0
3 150.131 114553.0
4 559.628 115350.0
5 666.085 120359.0
6 925.522 130035.0
7 1101.58 134702.0
8 1472.54 138914.0
9 1968.42 144947.0
10 2482.89 153371.0
11 3449.97 163161.0
12 4351.67 168284.0
13 5383.84 173748.0
14 5489.03 165324.0
15 5596.28 156445.0
16 6046.62 141646.0
17 6408.0 138345.0
18 7776.0 135385.0
19 17869.0 130263.0
20 35861.0 124912.0
!)
!)
!)
TF_ID 'Tvapor'      1.0 ! ( x
TF_BND 'POINT' 'POINT'
TF_TAB  15 ! (
1 10.1889 304.084
2 80.58 304.712
3 516.239 305.34
4 769.502 332.984
5 1003.9 353.403
6 1812.76 378.22
7 2808.14 403.979
8 3664.38 422.199
9 5263.73 437.592
10 5485.7 409.319
11 5824.63 385.759
12 6178.52 371.309
13 7636.81 359.372
14 13839.3 350.576
15 35421.5 336.126
!)
!)

```

```

TF_ID 'NAI' 1.0 ! ( x
TF_BND 'POINT' 'POINT'
TF_TAB 19 ! (
1 0.10411 1.42E-05
2 0.585785 7.86E-05
3 2.69002 0.000367659
4 12.779 0.00180528
5 74.3779 0.010244
6 404.566 0.0553931
7 696.289 0.141851
8 883.187 0.235357
9 1465.46 0.19407
10 2195.64 0.119821
11 3176.79 0.0467904
12 3618.15 0.0158108
13 3626.91 0.00588347
14 4274.78 0.00241101
15 5976.34 0.000757846
16 6824.32 0.00027529
17 8059.02 9.30E-05
18 14242.3 1.20E-05
19 26037.9 1.62E-06
!)
!)
TF_ID 'NAO' 1.0 ! ( x
TF_BND 'POINT' 'POINT'
TF_TAB 13 ! (
1 628.546 1.03E-06
2 672.114 7.61E-05
3 718.702 0.00658894
4 768.519 0.107488
5 821.79 2.12582
6 1606.28 28.6053
7 2483.19 19.4625
8 4389.47 25.1592
9 5190.11 15.5467
10 6785.8 2.93021
11 10144.6 0.984082
12 22673.0 0.232195
13 42856.5 0.0685862
!)
!)

#####
!
! / _ _ | | _ \ _ _ | _ _ _ _ _
! | ( _ | _ | | _ / _ _ / _ _ / _ _ / _ _
! \ _ | _ | | _ \ _ _ | _ \ _ _ \ _ _ \ _ _
! | _ _ /
#####

CF_INPUT

CF_ID 'Pressure (exp)' 401 TAB-FUN ! (
CF_UNITS 'Pa'
CF_SAI 1.0 0.0 0.0
CF_MSC 'Pressure'
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 EXEC-TIME 1.0 0.0
!)
CF_ID 'T Vapor (exp)' 402 TAB-FUN ! (
CF_UNITS 'K'
CF_SAI 1.0 0.0 0.0
CF_MSC 'Tvapor'
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 EXEC-TIME 1.0 0.0
!)
CF_ID 'NaI Mass (exp)' 403 TAB-FUN ! (

```



```

CVH_INPUT !(
!
! CSTF - containment vessel
! Env - environment volume
!
CV_ID          'CSTF'          1 !(
CV_TYP          'CTYP-2'
CV_THR          NONEQUIL          FOG          ACTIVE
CV_PAS          SEPARATE          ONLYATM          SUPERHEATED
CV_PTD          PVOL          1.145E5
CV_AAD          TATM          304.15
CV_NCG          4          RHUM          0.0
!              n          namgas          mass
!              1          'N2'          0.76245 ! 7.4632e-1 !0.767
!              2          'O2'          0.22774 ! 2.3368e-1 !0.233
3              'H2OV'          0.00981 ! 2.0000e-2
4 'H2'0.0
! 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 1
!!!'N2'          0.76245
!!!'O2'          0.22774
!!!'H2OV'        0.00981
CV_VAT          4 !n          cvz          cvvol
!              1          0.0          0.0
!              2          1.9          50.0
!              3          18.4          752.0
!              4          20.3          852.0
CV_SOU          4 !n          ctyp          interp          iessrc          idmat
1 mass          rate          tf          'O2SOURCE'          O2
2 te            rate          tf          'O2TEMP'          -1
3 mass          rate          tf          'N2SOURCE'          N2
4 te            rate          tf          'N2TEMP'          -1
!!!CV_SOU       1 !n          ctyp          interp          iessrc          srcname
!!!              1          AE          INTEGRAL          TF          'EXHEAT'
!)
CV_ID          'ENV'          2 !(
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
!)
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!              HS DATA          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!!
!!HS_INPUT !(
!!HS_ID          'top head'          1 !(
!!HS_GD          RECTANGULAR          NO
!!HS_EOD          18.4          0.0
!!HS_SRC          NO
!!HS_ND          7 !n n          xi tempin          matnam
!!              1 1          0.0 303.45 CARBON-STEEL
!!              2 2          0.0181 298.15 'fiberglass'
!!              3 3          0.02118 298.15 'fiberglass'

```

```

!!          4 4 0.02426 298.15 'fiberglass'
!!          5 5 0.02734 298.15 'fiberglass'
!!          6 6 0.03042 298.15 'fiberglass'
!!          7 7 0.0335 298.15
!!HS_LB      CalcCoefHS          'CSTF'          YES
!!HS_LBR      0.9          GRAY-GAS-A          20.3
!!HS_LBP      EXT          1.0          1.0
!!HS_LBS      63.0          7.62          7.62
!!HS_RB      TempTimeTF 'CSTF-TEMP'
!!HS_RBP      INT          0.0          0.0
!!HS_FT      OFF
!!!)
!!HS_ID      'walls-edge'          2 ! (
!!HS_GD      CYLINDRICAL          NO
!!HS_EOD      1.9          1.0
!!HS_SRC      NO
!!HS_ND      7 !n n          xi tempin          matnam
!!          1 1          3.81 303.45 CARBON-STEEL
!!          2 2 3.8329 298.15 'fiberglass'
!!          3 3 3.83798 298.15 'fiberglass'
!!          4 4 3.84306 298.15 'fiberglass'
!!          5 5 3.84814 298.15 'fiberglass'
!!          6 6 3.85322 298.15 'fiberglass'
!!          7 7 3.8583 298.15
!!HS_LB      CalcCoefHS          'CSTF'          YES
!!HS_LBR      0.9          GRAY-GAS-A          7.62
!!HS_LBP      EXT          1.0          1.0
!!HS_LBS      395.0          7.62          16.5
!!HS_RB      TempTimeTF 'CSTF-TEMP'
!!HS_RBP      INT          0.0          0.0
!!HS_FT      OFF
!!!)
!!HS_ID      'vert-int'          3 ! (
!!HS_GD      RECTANGULAR          NO
!!HS_EOD      0.0          1.0
!!HS_SRC      NO
!!HS_ND      2 !n n          xi tempin          matnam
!!          1 1          0.0 304.15 CARBON-STEEL
!!          2 2 3.4E-3 304.15
!!HS_LB      CalcCoefHS          'CSTF'          YES
!!HS_LBR      0.9          GRAY-GAS-A          3.81
!!HS_LBP      EXT          1.0          1.0
!!HS_LBS      232.0          7.62          7.62
!!HS_RB      CalcCoefHS          'CSTF'          YES
!!HS_RBR      0.9          GRAY-GAS-A          3.81
!!HS_RBP      EXT          1.0          1.0
!!HS_RBS      232.0          7.62          7.62
!!HS_FT      OFF
!!!)
!!HS_ID      'floor'          4 ! (
!!HS_GD      RECTANGULAR          NO
!!HS_EOD      0.000          -1.0E-7
!!! ORIGINAL --> HS_EOD          0.0435          -1.0E-7
!!HS_SRC      NO
!!HS_ND      7 !n n          xi tempin          matnam
!!          1 1          0.0 303.45 CARBON-STEEL
!!          2 2 0.0181 298.15 'fiberglass'
!!          3 3 0.02318 298.15 'fiberglass'
!!          4 4 0.02826 298.15 'fiberglass'
!!          5 5 0.03334 298.15 'fiberglass'
!!          6 6 0.03842 298.15 'fiberglass'
!!          7 7 0.0435 298.15
!!HS_LB      CalcCoefHS          'CSTF'          YES
!!HS_LBR      0.9          GRAY-GAS-A          20.3
!!HS_LBP      EXT          1.0          1.0
!!HS_LBS      45.604          7.62          7.62
!!HS_RB      TempTimeTF 'CSTF-TEMP'
!!HS_RBP      INT          0.0          0.0

```

```

!!HS_FT          OFF
!!!)
!!HS_ID          'horiz-int'          5 ! (
!!HS_GD          RECTANGULAR          NO
!!HS_EOD          1.9                  0.0
!!HS_SRC          NO
!!HS_ND          2 !n n          xi tempin          matnam
!!              1 1          0.0 304.15 CARBON-STEEL
!!              2 2 3.4E-3 304.15
!!HS_LB          CalcCoefHS          'CSTF'          YES
!!HS_LBR          0.9          GRAY-GAS-A          3.81
!!HS_LBP          EXT          1.0          1.0
!!HS_LBS          42.696          7.62          7.62
!!HS_RB          CalcCoefHS          'CSTF'          YES
!!HS_RBR          0.9          GRAY-GAS-A          3.81
!!HS_RBP          EXT          1.0          1.0
!!HS_RBS          42.696          7.62          7.62
!!HS_FT          OFF
!!!)
!!!)
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'          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 = CSTF CYLINDER WALLS

```

```

!
!      hsname      ishnum
HS_ID    'walls-edge'      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'      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    395.0      7.62      16.5 !3.8
!      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'      3 !( 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'      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      7.62
!      ibcr      ibvr      mteval
HS_RB    CalcCoefHS      'CSTF'      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      7.62
!      iftnum

```



```

HS_FT          OFF
!)
! HS 4 = BOTTOM HEAD
!
!           hsname          ishnum
HS_ID          'floor'          4 !( 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'          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          7.62
!           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'          5 !( 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'          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'          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
!)
!)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!              RN DATA      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

RN1_INPUT        0 ! (
!
!
RN1_DIM          20          3            22          6
RN1_DCHNORM      NONE
!
! ** AEROSOL PARAMETERS
! * 0.1e-6 = Lower bound for aerosol 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-8      1.0E-4      3670.0
!RN1_ASP          1.0E-8      5.0e-5      2500.0
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          0.99
!              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_MS01         2.5E-3      0.05        2.25        1.0E-5
RN1_MS01         1.0E-3      0.05        1.00        1.0E-5

RN1_DS          7 !n          ids          isde          ityp
1              'top head'      LHS          CEILING
2              'walls-edge'    LHS          WALL
3              'vert-int'      LHS          WALL
4              'floor'        LHS          FLOOR
5              'horiz-int'     LHS          FLOOR
6              'vert-int'      RHS          INACTIVE
7              'horiz-int'     RHS          INACTIVE

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/
     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, AB6 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' VAPOR 'NAI' 0.0 1.4E-4 TF 'ASOURCE2'
RN1_AS01 LOGNORMAL 5.44E-7 1.55
! )
! #####
RN2_INPUT
! #####
! )
!
! //// add NAC models
! iactiv
NAC_INPUT 0 ! (
! NaCL1 NaCL2 NaCL3 NaCL4 NaCL5
NAC_RNCLASS H2OA NA NAOH NA2O2 NA2O
!
!n CVHNAME FNA2O
NAC_ATMCH 1
1 'CSTF' 0.0000e+0
!!! !n CVHNAME FO2 FHEAT FNA2O FNA2O2 TOFF DAB
!!!NAC_PFIRES 1
!!! 1 'CSTF' 0.0 0.1 0.0 0.5 5400.0 0.0
NAC_SPRAY 1
!n CVHNAME HITE DME FNA2O2 SPRDT SOU-TYPE MASS-NAME THERM-NAME DROPVEL-NAME
1 'CSTF' 5.2100e+0 6.4000e-4 1.0000e+0 0.0 TF 'SPRAY-M' 'SPRAY-T' 'SPRAY-V'

!=====
! MELGEN Sensitivity input
!
! Sensitivity input includes specification of all sensitivity cases including
! model selection and uncertain parameters including
! uncertainty in physics models, accident sequence, and system operability.
!=====

!include '../..../shared-input/sensitivity.gen' 'melgensensitivity'

!#####

end program melgen

!#####
! END OF MELGEN INPUT
!#####

!#####
!
! MELCOR input
!
!#####

program melcor

```

```

#####

!=====
! MELCOR Base input
!=====

!block: 'melcorbase'

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          EXEC DATA          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

EXEC_INPUT !(
EXEC_TITLE 'Sensitivity test AB6'
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  10.0   0.01 10000.0  10.0 50000.0 1.0E10
           2    10.0  1.0 1.0E-3 10000.0  10.0 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 2.77E5
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          CF DATA          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

CF_INPUT !(
CF_HTML 4
  1 'Vessel Pressure' 'Pressure' 'Pressure (exp)'
  2 'Vapor Pressure' CVH-TVAP.1 'T Vapor (exp)'
  3 'NaI Mass' 'NaI Mass' 'NaI Mass (exp)'
  4 'NaO Mass' 'NaO Mass' 'NaO Mass (exp)'

!=====
! MELCOR Sensitivity input
!=====

!include '../shared-input/sensitivity.gen' 'melcorsensitivity'

#####

end program melcor

#####
! END OF MELCOR INPUT
#####

```


APPENDIX D. SOUTO INPUT DECKS

D.1. AB5

```
*m: SNAP:Symbolic Nuclear Analysis Package, Version 4.0.3, April 1, 2022
*m: PLUGIN:MELCOR Version 2.7.0
*m: CODE:MELCOR Version 2.2
*m: DATE:9/21/23
!
MEG_DIAGFILE '09mLgab5.dia'
MEG_OUTPUTFILE '09mLgab5.out'
MEG_RESTARTFILE '09ab5.rst'
PLOTFILE 'AB5_Souto_2x.PTF'
!
!*****
!'Sensitivity test AB5.09'
!*****
!
NOTEPAD++ ON
!
PROGRAM MELGEN
!
EXEC_INPUT
!
EXEC_TITLE 'Sensitivity test AB5.09'
!
EXEC_JOBID 'ab5-09'
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!      Tabular Functions Data      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
TF_INPUT
!
!
!cc: 2
!
!      tfname      tfscal      tfadcn
TF_ID      'EXTHEAT'      1.0      0.0
!
!      size
TF_TAB      5 !n      x      y
!      1      0.0      0.0
!      2      12.9      0.0
!      3      13.0      3.31E5
!      4      885.0      2.89E9
!      5      5.136E5      3.05E9
!
!
!cc: 5
!
!      tfname      tfscal      tfadcn
TF_ID      'ASOURCE'      1.0      0.0
!
!      size
TF_TAB      5 !n      x      y
!      1      0.0      0.0
!      2      12.95      0.0
!      3      13.0      1.0
!      4      885.0      1.0
!      5      886.0      0.0
!
!
!cc: 11
!
!      tfname      tfscal      tfadcn
TF_ID      'CPS-F'      1.0      0.0
!
!      ntfbdl      ntfbdu
TF_BND      CONST-BND      CONST-BND
!
!      size
TF_TAB      1 !n      x      y
```

```

1          0.0          753.0
!
!
!cc: 12
!          tfname          tfscal          tfadcn
TF_ID      'THC-F'          1.0          0.0
!          ntfbdl          ntfbdu
TF_BND      CONST-BND      CONST-BND
!          size
TF_TAB      1 !n          x          y
           1          0.0          0.0467
!
!
!cc: 13
!          tfname          tfscal          tfadcn
TF_ID      'RHO-F'          1.0          0.0
!          ntfbdl          ntfbdu
TF_BND      CONST-BND      CONST-BND
!          size
TF_TAB      1 !n          x          y
           1          0.0          96.0
!
!
!cc: 201
!          tfname          tfscal          tfadcn
TF_ID      'CSTF-TEMP'      1.0          0.0
!          size
TF_TAB      2 !n          x          y
           1          0.0          298.15
           2          5.14E5          298.15
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          Material Package          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
MP_INPUT
!
!
!cc: 0
!          matnam
MP_ID      'fibergLass'
!          size
MP_PRTF      3 !n          prop          itbprp          cfkey
           1          CPS          'CPS-F'
           2          THC          'THC-F'          TF
           3          RHO          'RHO-F'
!
!
!cc: 11
!          matnam
MP_ID      STAINLESS-STEEL
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          Noncondensable Gasses (NCG) Data          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
NCG_INPUT
!
!
!
!cc: 4
!          mname
NCG_ID      'N2'
!
!
!cc: 5
!          mname

```



```

NCG_ID      'O2'
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!      Decay Heat      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
DCH_INPUT
!
!      oprpow
DCH_OPW      10.0
DCH_CL  'XE'  DEFAULT
DCH_CL  'CS'  DEFAULT
DCH_CL  'BA'  DEFAULT
DCH_CL  'I2'  DEFAULT
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  'H2O' DEFAULT
DCH_CL  'CON' DEFAULT
DCH_CL  'CSI' DEFAULT
CVH_INPUT
!
!
!      cvname      icvnum
CV_ID      'CSTF'      1
!      icvtyp
CV_TYP      'CTYP-2'
!      icvthr      ipfsw      icvact
CV_THR      EQUIL      FOG      ACTIVE
!      itypth      ipora      vapor
CV_PAS      SEPARATE      ONLYATM      SUPERHEATED
!      ptdit      pvol
CV_PTD      PVOL      1.22E5
!      atmid      tatm
CV_AAD      TATM      302.25
!      nmmat      ncgid      tdew
CV_NCG      2      TDEW      289.15
!      n      namgas      mlfr
!      1      'N2'      0.767
!      2      'O2'      0.233

!      size
CV_VAT      4 !n      cvz      cvvol
!      1      0.0      0.0
!      2      1.9      50.0
!      3      18.4      752.0
!      4      20.3      852.0

!      size
CV_SOU      1 !n      ctyp      interp      iessrc      srcname
!      1      AE      INTEGRAL      TF      'EXTHEAT'
!
!
!      cvname      icvnum
CV_ID      'ENV'      2
!      icvtyp
CV_TYP      'CTYP-6'
!      icvthr      ipfsw      icvact
CV_THR      EQUIL      FOG      ACTIVE
!      itypth      ipora      water      vapor
CV_PAS      SEPARATE      POOLANDATM      SATURATED      SUPERHEATED
!      ptdit      pvol
CV_PTD      PVOL      1.01E5
!      atmid      tatm

```

```

CV_AAD          TATM          298.15
!              nmmt          ncgid          rhum
CV_NCG          2            RHUM          1.0
!              n            namgas          mlfr
!              1            'N2'          0.79
!              2            'O2'          0.21
!              bndid          vpol
CV_BND          VPOL          0.0
!              size
CV_VAT          2 !n          cvz          cvvol
!              1            0.0          0.0
!              2            1.0E10        1.0E10
!
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!      Heat Structures      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
HS_INPUT
!
!
!      hsname          ishnum
HS_ID          'top head'          1
!      igiom          iss
HS_GD          RECTANGULAR          NO
!      hsalt          alpha
HS_EOD          18.4          0.0
!      isrc
HS_SRC          NO
!      n size
HS_ND          7 3 !n n          xi          tempin          matnam
!              1 1          0.0          301.55 STAINLESS-STEEL
!              2 2 0.0181 300.9833333 'fibergLass'
!              3 7 0.0335          298.15
!      ibcl          ibvl          mteval
HS_LB          CalcCofHS          'CSTF'          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
!
!
!      hsname          ishnum
HS_ID          'waLLs-edge'          2
!      igiom          iss
HS_GD          CYLINDRICAL          NO
!      hsalt          alpha
HS_EOD          1.9          1.0
!      isrc
HS_SRC          NO
!      n size
HS_ND          7 3 !n n          xi          tempin          matnam
!              1 1          3.81          301.55 STAINLESS-STEEL
!              2 2 3.8329 300.9833333 'fibergLass'
!              3 7 3.8583          298.15
!      ibcl          ibvl          mteval
HS_LB          CalcCofHS          'CSTF'          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      395.0          7.62          16.5
!          ibcr           table
HS_RB      TempTimeTF    'CSTF-TEMP'
!          iflowr          cpfpr          cpfar
HS_RBP      INT           0.0           0.0
!          iftnum
HS_FT      OFF
!
!
!          hsname          ishnum
HS_ID      'vert-int'      3
!          igeom           iss
HS_GD      RECTANGULAR    NO
!          hsalt           alpha
HS_EOD      0.0           1.0
!          isrc
HS_SRC      NO
!      size
HS_ND      2 !n n          xi tempin          matnam
           1 1          0.0 302.25 STAINLESS-STEEL
           2 2 3.4E-3 302.25
!          ibcl           ibvl           mteval
HS_LB      CalcCoefHS      'CSTF'          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          7.62
!          ibcr           ibvr           mteval
HS_RB      CalcCoefHS      'CSTF'          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          7.62
!          iftnum
HS_FT      OFF
!
!
!          hsname          ishnum
HS_ID      'fLoor'          4
!          igeom           iss
HS_GD      RECTANGULAR    NO
!          hsalt           alpha
HS_EOD      0.0435          -1.0E-7
!          isrc
HS_SRC      NO
!      n size
HS_ND      7 3 !n n          xi          tempin          matnam
           1 1          0.0          301.55 STAINLESS-STEEL
           2 2 0.0181 300.9833333 'fibergLass'
           3 7 0.0435          298.15
!          ibcl           ibvl           mteval
HS_LB      CalcCoefHS      'CSTF'          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          7.62
!          ibcr           table
HS_RB      TempTimeTF    'CSTF-TEMP'
!          iflowr          cpfpr          cpfar
HS_RBP      INT           0.0           0.0
!          iftnum

```

```

HS_FT          OFF
!
!
!      hsname      ishnum
HS_ID      'horz-int'      5
!      igeom      iss
HS_GD      RECTANGULAR      NO
!      hsalt      alpha
HS_EOD      1.9      0.0
!      isrc
HS_SRC      NO
!      size
HS_ND      2 !n n      xi tempin      matnam
          1 1      0.0 302.25 STAINLESS-STEEL
          2 2 3.4E-3 302.25
!      ibcl      ibvl      mteval
HS_LB      CalcCoefHS      'CSTF'      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'      YES
!      emiswr      rmodr      pathr
HS_RBR      0.9      GRAY-GAS-A      3.81
!      iflowr      cpfpr      cpfal
HS_RBP      EXT      1.0      1.0
!      asurfr      clnr      bndzr
HS_RBS      42.696      7.62      7.62
!      iftnum
HS_FT          OFF
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!      Radionuclides      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!      iactv
RN1_INPUT      0
!      dft
RN1_DFT      1.86
!      numsec      numcmp      numcls      numca
RN1_DIM      20      1      16      6
!      iclnrm
RN1_DCHNORM      NONE
!      dmin      dmax      rhonom
RN1_ASP      1.0E-7      5.0E-5      2500.0
!      icoeff
RN1_ACOEF      CALANDWR
!      pgas1      pgas2      tgas1      tgas2
RN1_PT      1.0E5      2.13E5      298.0      581.15
!      chi      gamma      fslip      stick
RN1_MS00      1.5      2.25      1.37      1.0
!      chi      gamma      fslip      stick
RN1_MS01      1.0E-3      0.05      1.0      1.0E-5
!
!RN1_CC      jp xxxxxx conversion failed to properly set these, allowing defaults for now
!!      nstr      clsnam      cmpnm
!      1      XE      -1
!      2      CS      -1
!      3      BA      -1
!      4      I2      -1
!      5      TE      -1
!      6      RU      -1
!      7      MO      -1
!      8      CE      -1
!      9      LA      -1

```

```

!           10           UO2           -1
!           11           CD            -1
!           12           AG            -1
!           13           BO2           -1
!           14           H2O           -1
!           15           CON           -1
!           16           CSI           -1
!
!      size
RN1_DS      7 !n          ids          isde          ityp
!           1      'top head'          LHS          CEILING
!           2      'waLLs-edge'        LHS          WALL
!           3      'vert-int'          LHS          WALL
!           4      'fLoor'             LHS          FLOOR
!           5      'horz-int'          LHS          FLOOR
!           6      'vert-int'          RHS          INACTIVE
!           7      'horz-int'          RHS          INACTIVE
!
!      turbmodel      transmodel      imodel
RN1_TURB      2          2          0
!
!      size
RN1_SET      1 !n          ivolf          ivolt          elev          area
!           1          'ENV'          'ENV'          0.0          1.0
!
!      name      ivol      iphs      iclss      rfrs      xm      itab      cfnam
RN1_AS      'AS000' 'CSTF' VAPOR      'CS'      0.0 0.445      TF 'ASOURCE'
!
!      idist          geommm          gsd
RN1_AS01      LOGNORMAL          5.0E-7          1.5

RN2_INPUT
END PROGRAM MELGEN

!
!*****
!'Sensitivity test AB5.09'
!*****
!
MEL_DIAGFILE '09mLgab5.dia'
MEL_OUTPUTFILE '09mLcab5.out'
MEL_RESTARTFILE '09ab5.rst' NCYCLE -1
PLOTFILE 'AB5_Souto_2x.PTF'
MESSAGEFILE '09mLcab5.mes'
!
PROGRAM MELCOR
!
EXEC_INPUT
!
EXEC_TITLE 'Sensitivity test AB5.09'
!
EXEC_CPULEFT 10.0
!
EXEC_CPULIM 2500.0
!
EXEC_JOBID 'ab5-09'
!
!      size
EXEC_TIME      8 !n      time      dtmax      dtmin      dedit      dtplot      dtrest      dcrest
!           1          0.0      10.0      0.01      10000.0      10.0      50000.0      1.0E10
!           2          10.0      10.0      0.01      10000.0      10.0      50000.0      1.0E10
!           3          30.0      10.0      0.01      10000.0      10.0      50000.0      1.0E10
!           4          60.0      10.0      0.01      10000.0      40.0      50000.0      1.0E10
!           5          300.0      10.0      0.01      10000.0      50.0      50000.0      1.0E10
!           6          600.0      10.0      0.01      10000.0      100.0      50000.0      1.0E10
!           7          1200.0      10.0      0.01      12000.0      400.0      50000.0      1.0E10
!           8          4800.0      1000.0      0.01      12000.0      400.0      50000.0      1.0E10
!
EXEC_TEND 5.14E5
END PROGRAM MELCOR

```

D.2. AB6

```
!*****
!*****
! $Id$
! Abcove AB6
! reference case: 10 sections aerosol bin
!
! Developed by:
! Sandia National Laboratories
!
! Revision History
! -----
! 11.14.22 input refactored @dkeesli
!
! -----
!
! References:
! Assessment Document SVN URL: https://svn-melcor.sandia.gov/svn/melcor-II/documentation/trunk/Assessments/ABCOV
! MELCOR 1.8.2 report SVN URL: https://svn-melcor.sandia.gov/svn/melcor-II/documentation/trunk/Assessments/ABCOV
!
!
!*****
!*****
!
! MELGEN and MELGEN/MELCOR common file names
!
!*****
MEG_DIAGFILE      'abcove_ab6_10sect.gdia'
MEL_DIAGFILE      'abcove_ab6_10sect.dia'
MEG_OUTPUTFILE    'abcove_ab6_10sect.gout'
MEL_OUTPUTFILE    'abcove_ab6_10sect.out'
! MEL_HTMLFILE     ab6-10sect.htm
MEG_RESTARTFILE   'abcove_ab6_10sect.rst'
MEL_RESTARTFILE   'abcove_ab6_10sect.rst' -1
PLOTFILE          'abcove_ab6_10sect.ptf'
MESSAGEFILE       'abcove_ab6_10sect.mes'
STATUSFILE        'MELSTT'
STOPFILE          'MELSTP'
WRITENEWINP       'MELGIN.CAN'
!DefaultDirectory '.\output'
allowreplace
commentblock 10sect

#####
!
! MELGEN input
!
#####

program melgen

#####

!=====
! MELGEN Base input
!
! Base input includes specification of all plant systems and severe accident
! physics.
!=====

!block: 'melgenbase'

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          EXEC DATA          !
```

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

EXEC_INPUT !(
EXEC_TITLE 'Sensitivity test AB6'
EXEC_DTIME 1.0E-3
EXEC_GLOBAL_DFT 2.0 ! global flag for 2.0 is used.
EXEC_JOBID 'REF'
EXEC_PLOT 12 !(
1 RN1-TYCLAIR(CS,'CTYP-2','TOT')
  2 RN1-TYCLAIR(CSI,'CTYP-2','TOT')
  3 RN1-ADEP('top head',LHS,'CS',TOT)
  4 RN1-ADEP('walls-edge',LHS,'CS',TOT)
  5 RN1-ADEP('vert-int',LHS,'CS',TOT)
  6 RN1-ADEP('floor',LHS,'CS',TOT)
  7 RN1-ADEP('horiz-int',LHS,'CS',TOT)
  8 RN1-ADEP('top head',LHS,'CSI',TOT)
  9 RN1-ADEP('walls-edge',LHS,'CSI',TOT)
 10 RN1-ADEP('vert-int',LHS,'CSI',TOT)
 11 RN1-ADEP('floor',LHS,'CSI',TOT)
 12 RN1-ADEP('horiz-int',LHS,'CSI',TOT)
!)
!)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          TF DATA          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

TF_INPUT !(
TF_ID      'EXHEAT'          1.0          0.0 !(
TF_TAB      5 !n              x              y
              1              0.0              0.0
              2              619.9              0.0
              3              620.0             29400.0
              4              5400.0             2.86E9
              5              2.77E5             3.0E9
!)
! NaI source (class 2)
TF_ID      'ASOURCE1'       1.0          0.0 !(
TF_TAB      6 !n              x              y
              1              0.0              0.0
              2              619.95             0.0
              3              620.0              1.0
              4              5400.0             1.0
              5              5401.0             0.0
              6              2.77E5             0.0
!)
! NaOx source (class 16)
TF_ID      'ASOURCE2'       1.0          0.0 !(
TF_TAB      4 !n              x              y
              1              0.0              1.0
              2              3000.0             1.0
              3              3001.0             0.0
              4              2.77E5             0.0
!)
TF_ID      'DECAY'          1.0          0.0 !(
TF_TAB      2 !n              x              y
              1              0.0              0.0
              2              2.77E5             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      5.14E5    298.15
!)
!)
TF_ID 'Pressure'      1.0 ! ( x
TF_BND 'POINT'      'POINT'
TF_TAB  20 ! (
1 10.0 114212.0
2 42.6827 114326.0
3 150.131 114553.0
4 559.628 115350.0
5 666.085 120359.0
6 925.522 130035.0
7 1101.58 134702.0
8 1472.54 138914.0
9 1968.42 144947.0
10 2482.89 153371.0
11 3449.97 163161.0
12 4351.67 168284.0
13 5383.84 173748.0
14 5489.03 165324.0
15 5596.28 156445.0
16 6046.62 141646.0
17 6408.0 138345.0
18 7776.0 135385.0
19 17869.0 130263.0
20 35861.0 124912.0
!)
!)
!)
TF_ID 'Tvapor'      1.0 ! ( x
TF_BND 'POINT'      'POINT'
TF_TAB  15 ! (
1 10.1889 304.084
2 80.58 304.712
3 516.239 305.34
4 769.502 332.984
5 1003.9 353.403
6 1812.76 378.22
7 2808.14 403.979
8 3664.38 422.199
9 5263.73 437.592
10 5485.7 409.319
11 5824.63 385.759
12 6178.52 371.309
13 7636.81 359.372
14 13839.3 350.576
15 35421.5 336.126
!)
!)
TF_ID 'NAI'      1.0 ! ( x
TF_BND 'POINT'      'POINT'
TF_TAB  19 ! (
1 0.10411 1.42E-05
2 0.585785 7.86E-05
3 2.69002 0.000367659
4 12.779 0.00180528
5 74.3779 0.010244
6 404.566 0.0553931
7 696.289 0.141851

```



```

8 883.187 0.235357
9 1465.46 0.19407
10 2195.64 0.119821
11 3176.79 0.0467904
12 3618.15 0.0158108
13 3626.91 0.00588347
14 4274.78 0.00241101
15 5976.34 0.000757846
16 6824.32 0.00027529
17 8059.02 9.30E-05
18 14242.3 1.20E-05
19 26037.9 1.62E-06
!)
!)
TF_ID 'NAO' 1.0 !( x
TF_BND 'POINT' 'POINT'
TF_TAB 13 !(
1 628.546 1.03E-06
2 672.114 7.61E-05
3 718.702 0.00658894
4 768.519 0.107488
5 821.79 2.12582
6 1606.28 28.6053
7 2483.19 19.4625
8 4389.47 25.1592
9 5190.11 15.5467
10 6785.8 2.93021
11 10144.6 0.984082
12 22673.0 0.232195
13 42856.5 0.0685862
!)
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! CF DATA !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

CF_INPUT

CF_ID 'Pressure (exp)' 401 TAB-FUN !(
CF_UNITS 'Pa'
CF_SAI 1.0 0.0 0.0
CF_MSC 'Pressure'
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 EXEC-TIME 1.0 0.0
!)
CF_ID 'T Vapor (exp)' 402 TAB-FUN !(
CF_UNITS 'K'
CF_SAI 1.0 0.0 0.0
CF_MSC 'Tvapor'
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 EXEC-TIME 1.0 0.0
!)
CF_ID 'NaI Mass (exp)' 403 TAB-FUN !(
CF_UNITS 'Kg'
CF_SAI 1.0 0.0 0.0
CF_MSC 'NAI'
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 EXEC-TIME 1.0 0.0
!)
CF_ID 'NaO Mass (exp)' 404 TAB-FUN !(
CF_UNITS 'Kg'
CF_SAI 1.0 0.0 0.0
CF_MSC 'NAO'
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 EXEC-TIME 1.0 0.0
!)
CF_ID 'Pressure' 501 EQUALS !(

```

```

CF_UNITS 'Pa'
CF_SAI 1.0 0.0 0.0
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 CVH-P('CSTF') 1.0 0.0
!)
CF_ID 'T Vapor' 502 EQUALS ! (
CF_UNITS 'K'
CF_SAI 1.0 0.0 0.0
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 CVH-TVAP('CSTF') 1.0 0.0
!)
CF_ID 'NaI Mass' 503 EQUALS ! (
CF_UNITS 'Kg'
CF_SAI 1.0 0.0 0.0
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 RN1-TYCLAIR('CSI','CTYP-2','TOT') 1.0 0.0
!)
CF_ID 'NaO Mass' 504 EQUALS ! (
CF_UNITS 'Kg'
CF_SAI 1.0 0.0 0.0
CF_ARG 1 ! NARG CHARG ARSCAL ARADCN
1 RN1-TYCLAIR('CS','CTYP-2','TOT') 1.0 0.0
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! MP DATA !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

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 STAINLESS-STEEL
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! NCG DATA !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

NCG_INPUT ! (
NCG_ID 'N2'
NCG_ID 'O2'
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! DCH DATA !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

DCH_INPUT ! (
DCH_RCT PWR
DCH_SHT TIME 0.0
DCH_OPW 2.68597E9
DCH_DPW TF 'DECAY'
DCH_FPW 1.7387E9 8.3423E8 1.1304E8
!DCH Classes
! (
DCH_CL 'XE' DEFAULT
DCH_CL 'CS' DEFAULT
DCH_CL 'BA' DEFAULT
DCH_CL 'I2' DEFAULT
DCH_CL 'TE' DEFAULT
DCH_CL 'RU' DEFAULT
DCH_CL 'MO' DEFAULT
DCH_CL 'CE' DEFAULT

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DCH_CL 'LA'      DEFAULT
DCH_CL 'UO2'     DEFAULT
DCH_CL 'CD'      DEFAULT
DCH_CL 'AG'      DEFAULT
DCH_CL 'BO2'     DEFAULT
DCH_CL 'H2O'     DEFAULT
DCH_CL 'CON'     DEFAULT
DCH_CL 'CSI'     DEFAULT
!)
DCH_NRM          YES
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!      CVH DATA      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

CVH_INPUT ! (
!
! CSTF - containment vessel
! Env - environment volume
!
CV_ID          'CSTF'          1 ! (
CV_TYP          'CTYP-2'
CV_THR          EQUIL          FOG          ACTIVE
CV_PAS          SEPARATE        ONLYATM      SUPERHEATED
CV_PTD          PVOL           1.145E5
CV_AAD          TATM           304.15
CV_NCG          2              TDEW          285.35
!
!              n              namgas          mass
!              1              'N2'           0.761
!              2              'O2'           0.239
CV_VAT          4 !n          cvz          cvvol
!              1              0.0          0.0
!              2              1.9          50.0
!              3              18.4         752.0
!              4              20.3         852.0
CV_SOU          1 !n          ctyp          interp          iessrc          srcname
!              1              AE          INTEGRAL          TF          'EXHEAT'
!)
CV_ID          'ENV'          2 ! (
CV_TYP          'CTYP-6'
CV_THR          EQUIL          FOG          ACTIVE
CV_PAS          SEPARATE        POOLANDATM    SATURATED    SUPERHEATED
CV_PTD          PVOL           1.01E5
CV_AAD          TATM           298.15
CV_NCG          2              RHUM          1.0
!
!              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              1.0E10        1.0E10
!)
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!      HS DATA      !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

HS_INPUT ! (
HS_ID          'top head'          1 ! (
HS_GD          RECTANGULAR          NO
HS_EOD          18.4          0.0
HS_SRC          NO
HS_ND          7 !n n          xi tempin          matnam
!              1 1          0.0 303.45 STAINLESS-STEEL

```

```

2 2 0.0181 298.15 'fiberglass'
3 3 0.02118 298.15 'fiberglass'
4 4 0.02426 298.15 'fiberglass'
5 5 0.02734 298.15 'fiberglass'
6 6 0.03042 298.15 'fiberglass'
7 7 0.0335 298.15
HS_LB CalcCoefHS 'CSTF' YES
HS_LBR 0.9 GRAY-GAS-A 20.3
HS_LBP EXT 1.0 1.0
HS_LBS 63.0 7.62 7.62
HS_RB TempTimeTF 'CSTF-TEMP'
HS_RBP INT 0.0 0.0
HS_FT OFF
!)
HS_ID 'walls-edge' 2 ! (
HS_GD CYLINDRICAL NO
HS_EOD 1.9 1.0
HS_SRC NO
HS_ND 7 !n n xi tempin matnam
1 1 3.81 303.45 STAINLESS-STEEL
2 2 3.8329 298.15 'fiberglass'
3 3 3.83798 298.15 'fiberglass'
4 4 3.84306 298.15 'fiberglass'
5 5 3.84814 298.15 'fiberglass'
6 6 3.85322 298.15 'fiberglass'
7 7 3.8583 298.15
HS_LB CalcCoefHS 'CSTF' YES
HS_LBR 0.9 GRAY-GAS-A 7.62
HS_LBP EXT 1.0 1.0
HS_LBS 395.0 7.62 16.5
HS_RB TempTimeTF 'CSTF-TEMP'
HS_RBP INT 0.0 0.0
HS_FT OFF
!)
HS_ID 'vert-int' 3 ! (
HS_GD RECTANGULAR NO
HS_EOD 0.0 1.0
HS_SRC NO
HS_ND 2 !n n xi tempin matnam
1 1 0.0 304.15 STAINLESS-STEEL
2 2 3.4E-3 304.15
HS_LB CalcCoefHS 'CSTF' YES
HS_LBR 0.9 GRAY-GAS-A 3.81
HS_LBP EXT 1.0 1.0
HS_LBS 232.0 7.62 7.62
HS_RB CalcCoefHS 'CSTF' YES
HS_RBR 0.9 GRAY-GAS-A 3.81
HS_RBP EXT 1.0 1.0
HS_RBS 232.0 7.62 7.62
HS_FT OFF
!)
HS_ID 'floor' 4 ! (
HS_GD RECTANGULAR NO
HS_EOD 0.0435 -1.0E-7
HS_SRC NO
HS_ND 7 !n n xi tempin matnam
1 1 0.0 303.45 STAINLESS-STEEL
2 2 0.0181 298.15 'fiberglass'
3 3 0.02318 298.15 'fiberglass'
4 4 0.02826 298.15 'fiberglass'
5 5 0.03334 298.15 'fiberglass'
6 6 0.03842 298.15 'fiberglass'
7 7 0.0435 298.15
HS_LB CalcCoefHS 'CSTF' YES
HS_LBR 0.9 GRAY-GAS-A 20.3
HS_LBP EXT 1.0 1.0
HS_LBS 45.604 7.62 7.62
HS_RB TempTimeTF 'CSTF-TEMP'

```

```

HS_RBP          INT          0.0          0.0
HS_FT           OFF
!)
HS_ID           'horiz-int'          5 ! (
HS_GD           RECTANGULAR          NO
HS_EOD          1.9          0.0
HS_SRC          NO
HS_ND           2 !n n          xi tempin          matnam
                1 1          0.0 304.15 STAINLESS-STEEL
                2 2 3.4E-3 304.15
HS_LB           CalcCoefHS          'CSTF'          YES
HS_LBR          0.9          GRAY-GAS-A          3.81
HS_LBP          EXT          1.0          1.0
HS_LBS          42.696          7.62          7.62
HS_RB           CalcCoefHS          'CSTF'          YES
HS_RBR          0.9          GRAY-GAS-A          3.81
HS_RBP          EXT          1.0          1.0
HS_RBS          42.696          7.62          7.62
HS_FT           OFF
!)
!)

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          RN DATA          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

RN1_INPUT          0 ! (
!
! 20 = Number of sections, 2 = Number of aerosol components
! 1 = Number of tabular aerosol sources
! Note that number of sections used was chosen based on the original deck developed
! It is not expected that significant difference in results if default number sections used (10)
!
! *** NaI AEROSOL COMPONENT 1 ***
! * 1 = Volume for aerosol source
! * 2 = Atmosphere to received aerosol mass
! * 16 = Class of aerosol (we will assume that NaI belongs to class 16)
! * 0. = Radioactive fraction of source
! * 1.4e-4 = Mass rate
! * 6 = Tabular function for mass rate
! * 2 = Log-normal distribution
!
!          dft
! RN1_DFT          1.86 ! comment out because EXEC GLOBAL_DFT 2.0 is used
!
((20sect
RN1_DIM          20          2          16          6
))
((10sect
RN1_DIM          10          2          16          6
))
RN1_DCHNORM          NONE
RN1_CLS 'RNCLS01' 'CSI'          2 !n          nclsd          xmrat
                1          'CS'          1.0
                2          'I2'          1.0
!
! ** AEROSOL PARAMETERS
! * 0.1e-6 = Lower bound for aerosol 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_ACOEF          CALANDWR

```

```

RN1_PT      50000.0      2.0E6      280.0      700.0
RN1_MS00      1.5      2.25      1.37      1.0      ! from SAND94-2166
RN1_MS01      1.0E-3      0.05      1.0      1.0E-5      ! from SAND94-2166
RN1_CC
!
      nstr      clsnam      cmpnm
      1      'XE'      1
      2      'CS'      1
      3      'BA'      1
      4      'I2'      1
      5      'TE'      1
      6      'RU'      1
      7      'MO'      1
      8      'CE'      1
      9      'LA'      1
     10      'UO2'      1
     11      'CD'      1
     12      'AG'      1
     13      'BO2'      1
     14      'H2O'      1
     15      'CON'      1
     16      'CSI'      2

RN1_DS      7 !n      ids      isde      ityp
      1      'top head'      LHS      CEILING
      2      'walls-edge'      LHS      WALL
      3      'vert-int'      LHS      WALL
      4      'floor'      LHS      FLOOR
      5      'horiz-int'      LHS      FLOOR
      6      'vert-int'      RHS      INACTIVE
      7      'horiz-int'      RHS      INACTIVE

RN1_SET      1 !n      ivolf      ivolt      elev      area
      1      'ENV'      'ENV'      0.0      1.0

!
! *** AEROSOL SOURCES
! *
! *** NaOx AEROSOL COMPONENT 2 ***
! * 1 = Volume for aerosol source
! * 2 = Atmosphere to received aerosol mass
! * 2 = Class of aerosol (Na belongs to alkali metals, class 2)
! * 0. = Radioactive fraction of source
! * 7.79e-2 = Mass rate
! * 5 = Tabular function for mass rate
! * 2 = Log-normal distribution
!
RN1_AS      'AS000'      'CSTF'      VAPOR      'CS'      0.0 0.0779      TF      'ASOURCE1'
RN1_AS01      LOGNORMAL      5.0E-7      2.0
RN1_AS      'AS002'      'CSTF'      VAPOR      'CSI'      0.0 1.4E-4      TF      'ASOURCE2'
RN1_AS01      LOGNORMAL      5.44E-7      1.55
!))

!=====
! MELGEN Sensitivity input
!
! Sensitivity input includes specification of all sensitivity cases including
! model selection and uncertain parameters including
! uncertainty in physics models, accident sequence, and system operability.
!=====

!include '../shared-input/sensitivity.gen' 'melgensensitivity'

#####

end program melgen

#####
! END OF MELGEN INPUT
#####

```

```

#####
!
! MELCOR input
!
#####

program melcor

#####

!=====
! MELCOR Base input
!=====

!block: 'melcorbase'

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          EXEC DATA          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

EXEC_INPUT !(
EXEC_TITLE 'Sensitivity test AB6'
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  10.0   0.01 10000.0  10.0 50000.0 1.0E10
            2    10.0  1.0 1.0E-3 10000.0  10.0 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 2.77E5
! )

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          CF DATA          !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

CF_INPUT !(
CF_HTML 4
1 'Vessel Pressure' 'Pressure' 'Pressure (exp)'
2 'Vapor Pressure' CVH-TVAP.1 'T Vapor (exp)'
3 'NaI Mass' 'NaI Mass' 'NaI Mass (exp)'
4 'NaO Mass' 'NaO Mass' 'NaO Mass (exp)'

!=====
! MELCOR Sensitivity input
!=====

!include '../..'/shared-input/sensitivity.gen' 'melcorsensitivity'

#####

end program melcor

#####
! END OF MELCOR INPUT
#####

```


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