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Metal Fire Implications for Advanced Reactors, Part 2: PIRT Results

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CONTENTS

FIGURES

TABLES

NOMENCLATURE

ABTR	Advanced Breeder Test Reactor
CFD	Computational Fluid Dynamics
IHTS	Intermediate Heat Transport System
IHX	Intermediate Heat Exchanger
LDRD	Laboratory Directed Research and Development
PCHE	Printed Circuit Heat Exchanger
PHTS	Primary Heat Transport System
PIRT	Phenomena Identification and Ranking Table
SNL	Sandia National Laboratories
TRU	Transuranic

Chemical Formulas

CO_2	Carbon Dioxide
Mo	Molybdenum
Na	Sodium
Na_2O	Sodium Oxide
Na_2O_2	Sodium Peroxide
$S\text{-}CO_2$	Supercritical Carbon Dioxide
U	Uranium

Symbols

atm	Standard Atmosphere
°C	Degrees Centigrade
g	Gram
K	Degrees Kelvin
kg	Kilo-gram
s	Second
m	Meter
MWe	Megawatt Electric
MWt	Megawatt Thermal
Pa	Pascal
W	Watt

1 INTRODUCTION

1.1 Overview

This report documents the results of a Phenomena Identification and Ranking Table (PIRT) exercise performed at Sandia National Laboratories (SNL) as well as the experimental and modeling program that have been designed based on the PIRT results.

A PIRT exercise is a structured and facilitated expert elicitation process. In this case, the expert panel was comprised of nine recognized fire science and aerosol experts. The objective of a PIRT exercise is to identify phenomena associated with the intended application and to then rank the current state of knowledge relative to each identified phenomenon. In this particular PIRT exercise the intended application was sodium fire modeling related to sodium-cooled advanced reactors.

The panel was presented with two specific fire scenarios, each based on a hypothetical sodium leak in an Advanced Breeder Test Reactor (ABTR) design. For both scenarios the figure of merit was the ability to predict the thermal and aerosol insult to nearby equipment (i.e. heat exchangers and other electrical equipment). When identifying phenomena of interest, and in particular when ranking phenomena importance and the adequacy of existing modeling tools and data, the panel was asked to subjectively weigh these factors in the context of the specified figure of merit.

Given each scenario, the panel identified all those related phenomena that are of potential interest to an assessment of the scenario using fire modeling tools to evaluate the figure of merit. Each phenomenon is then ranked relative to its importance in predicting the figure of merit. Each phenomenon is then further ranked for the existing state of knowledge with respect to the ability of existing modeling tools to predict that phenomena, the underlying base of data associated with the phenomena, and the potential for developing new data to support improvements to the existing modeling tools.

For this PIRT two hypothetical sodium leak scenarios were evaluated for the ABTR design. The first scenario was a leak in the hot side of the intermediate heat transport system (IHTS) resulting in a sodium pool fire. The second scenario was a leak in the cold side of the IHTS resulting in a sodium spray fire.

2 OVERVIEW OF THE PHENOMENA IDENTIFICATION RANKING TABLE PROCESS APPLIED

2.1 Background

A PIRT exercise is a formal expert elicitation process with the final output being the ranking tables. The goal of the PIRT exercise was to develop input for the Metal Fire Laboratory Directed Research and Development (LDRD) experimental program. The input from this exercise has been used for the design of the discovery sodium fire experiments. This data will be used to develop sodium fire modeling codes. This PIRT process provides insight to those areas of sodium fire modeling that experts consider to be (1) important, (2) poorly understood or poorly dealt with given the current state of the art, and (3) amenable to additional research.

2.2 Selection of Panelists

Members of the PIRT panel were identified by the SNL staff. The selected panelists represent a range of specific expertise areas and backgrounds. Metal fire/combustion and advanced reactor technology are highly specialized fields of expertise, and the number of individuals in the world with suitable expertise, experience, and recognition is limited.

The individuals who made up the expert panel include eight SNL technical staff members and one University of Buffalo Professor. The panel members were:

- Amalia R. Black
- John E. Brockmann
- Tze Yao (T.Y.) Chu
- Paul E. DesJardin
- Stefan P. Domino
- Kenneth L. Erickson
- John C. Hewson
- Dana A. Powers

The three SNL staff technical area experts were:

- Thomas K. Blanchat
- Jeanne A. Dion
- Gary E. Rochau

The two SNL staff facilitators were:

- Vernon F. Nicolette
- Tara J. Olivier

All of the selected panelists and technical area experts are widely recognized and published. Appendix A presents the resumes supplied by each PIRT participant.

2.3 The PIRT Process Applied

This section describes the PIRT process as exercised for this project. The scenarios were evaluated together as most of the identified phenomena were the same if not similar. For the two fire scenario, the panelists were asked to complete the following stages of assessment:

1. Understand the given fire scenario and figure of merit, and ask clarifying questions as needed.
2. Identify phenomena of interest.
3. Rank the importance of each phenomenon in the context of the figure of merit.
4. Rank the state of knowledge of each phenomenon relative to the model adequacy, code adequacy, available input data, feasibility of obtaining new input data, available validation data, and the feasibility of obtaining new validation data. This step was only performed on those phenomena that were ranked with a high or medium importance.

To complete the first stage of analysis, the given fire scenario was presented to the panelists. Panelists were given an opportunity to ask any clarifying questions, and the technical area experts supporting the process often played a key role in answering such questions. Once a list of phenomena had been developed, the next stage of the analysis was to rank each phenomenon for importance relative to the figure of merit. The panel was asked to rank phenomena importance according to the descriptors provided in Table 2-1.

Table 2-1: Phenomena importance ranking definitions

Descriptor:	Definition:
High (H)	First order importance to figure of merit of interest.
Medium (M)	Secondary importance to figure of merit of interest.
Low (L)	Negligible importance to figure of merit of interest. Not necessary to model this parameter for this application.
Uncertain (U)	Potentially important. Importance should be explored through sensitivity study and/or discovery experiments and the PIRT revised accordingly.

The state of knowledge rankings were performed next on those phenomena that were ranked with a high importance ranking as well as most of the phenomena ranked with a medium importance ranking. There were six categories ranked for each phenomenon in respect to the state of knowledge. The first category was the assessment of model adequacy. This was meant as the general adequacy of existing fire modeling tools to meet the needs for modeling each identified phenomenon. This stage also includes ranking the code adequacy, which is specific to actual computer code adequacy. The descriptors for model and code adequacy are shown below in Table 2-2. The panelists were then asked to rank the adequacy of existing data needed to support model development and model validation. These descriptors are shown in Table 2-3. During the last stages the experts were to rank the feasibility of obtaining new model input and validation data if the existing data adequacy were ranked as anything other than “high”. The description for this stage of the state of knowledge rankings are defined in Table 2-4.

Table 2-2: Model adequacy ranking definitions

Descriptor:	Definition:
High (H)	At least one mature physics-based or correlation-based model is available that is believed to adequately represent the phenomenon over the full parameter space of the applications.
Medium (M)	Significant discovery activities have been completed. At least one candidate model form or correlation form has emerged that is believed to nominally capture the phenomenon over some portion of the application parameter space.
Low (L)	No significant discovery activities have occurred and model form is still unknown or speculative.
Uncertain (U)	The panel is unaware of the existing state of fire modeling tools with respect to this phenomenon.

Table 2-3: Data adequacy descriptors for existing model input and validation data

Descriptor:	Definition:
High (H)	A high resolution database (e.g., validation grade data set) exists, or a highly reliable assessment can be made based on existing knowledge. Data needed are readily available.
Medium (M)	Existing database is of moderate resolution, or not recently updated. Data are available but are not ideal due to age or questions of fidelity. Moderately reliable assessments of models can be made based on existing knowledge.
Low (L)	No existing database or low-resolution database in existence. Assessments cannot be made with even moderate reliability based on existing knowledge.

Table 2-4: Data adequacy descriptors for the potential to develop new data to support model development and validation.

Descriptor:	Definition:
High (H)	Data needed are readily obtainable based on existing experimental capabilities.
Medium (M)	Data would be obtainable but would require moderate, readily attainable extensions to existing capabilities.
Low (L)	Data are not readily obtainable and/or would require significant development of new capabilities.

3 PIRT SCENARIO DESCRIPTIONS

As mentioned above, this PIRT exercise consisted of two fire scenarios related to the ABTR design. The first scenario is a sodium leak in the hot side of the IHTS resulting in a sodium pool fire. The second scenario is a sodium leak in the cold side of the IHTS resulting in a sodium spray fire. This section explains the details of these two scenarios that were presented to the panel. All of the information about the design of the ABTR was taken from the *Advanced Burner Test Reactor Preconceptual Design Report* [1].

The ABTR design was chosen for this exercise for the following reasons:

- the design supports the development of prototype full scale Advanced Burner Reactors
- design aspects are similar to previous sodium cooled reactors, and
- details of the design are readily available.

The ABTR is a pool type sodium cooled reactor whose characteristics are listed in Table 3-1. The ABTR utilizes a pool-type primary cooling system where the reactor core, primary pumps, intermediate heat exchanger (IHX), and direct reactor auxiliary cooling system heat exchangers are submerged in a pool of liquid sodium.

Table 3-1: ABTR Design Parameters [1]

Reactor Power	250 MWt, 95 MWe
Coolant	Sodium
Coolant Temperature, Inlet/Outlet	355°C/510°C
Driver Fuel	Reference: Metal (~20% TRU, 80% U) Backup: Oxide
Cladding and Duct Material	HT-9
Cycle Length	4 Months
Plant Life	30 years with the expectation of life extension
Reactor Vessel Size	5.8 m diameter, 16 m height
Structural and Piping Material	Austenitic Stainless Steel
Primary Pump	Reference: Electromagnetic Backup: Mechanical (centrifugal)
Power Conversion Cycle	Reference: Supercritical CO_2 Brayton Backup: Steam Rankine
Thermal Efficiency	38%

The hot primary sodium transfers heat to the secondary sodium via a shell-in-tube IHX. The primary sodium is re-circulated with pumps through the core again. The secondary sodium travels through pipes to the auxiliary room where the heat exchangers are located for the power generation production. Two forms of power generation are being considered: a Brayton cycle supercritical carbon dioxide (S-CO_2) system and a Rankine cycle steam system.

The containment building and the passage ways used to transport the fuel assemblies to and from the reactor are inerted to prevent oxygen reactions with sodium. The auxiliary room containing the heat exchangers for power generation and the intermediate loop pumps are not inerted.

3.1 Details of Scenario 1: Sodium Pool Fire in Hot Leg

The first fire scenario is a postulated leak in the hot side of the IHTS, which results in a sodium pool fire. The IHTS circulates the secondary sodium coolant, which transfers heat between the primary heat transport system (PHTS) and the S-CO_2 power generation system. The PHTS transfers heat to the IHTS through a shell-in-tube sodium to sodium intermediate heat exchanger (IHX). The secondary sodium is heated in the IHX, exits the reactor containment and then travels to the S-CO_2 production facility (located within the reactor building). A compact heat exchanger design, called the printed circuit heat exchanger (PCHE), is used for sodium to S-CO_2 heat transfer. After the secondary sodium exits the PCHEs, an electromagnetic pump (EM) circulates the sodium back to the cold side of the IHX in the reactor containment. The major components are the EM pump, PCHE, sodium storage tank, and the piping that connects these components to each other and the IHX [1].

The IHX has secondary sodium flowing through tubes and primary sodium in the shell side. The tubes are made from modified 9Cr-1Mo steel while the other components are made from austenitic steel. Dissimilar metal welds are required since the secondary sodium flows to the IHTS pipes.

The PCHEs are compact counter flow heat exchanger designs where sodium and CO_2 liquid flow through micro-etched channels in 316 stainless steel sheets which have been welded together. Each of these heat exchangers is 1m long, by 0.6 m wide, by 0.6 m high and weighs 1.73 tons with a channel void fraction of 0.309. All IHTS pipes are made from 304 stainless steel (40.6 cm outer diameter and 1.27 cm wall thickness) and are enclosed in secondary piping.

The specifications for the leak in Scenario 1 are described here. For this scenario the panel considered a leak in the hot leg of the secondary system as shown in Figure 3.1. The secondary sodium characteristics are:

Temperature: 488°C
Pressure: ~1 atm
Density: ~ 900kg/m^3
Pipe Flow Rate: 628 kg/s
Pipe Flow Velocity: 5.2 m/s
Leak Flow Velocity: 15 m/s
Leak Flow Rate: ~5 kg/s

The figure of merit for this scenario is the ability to predict the thermal and aerosols insult to nearby equipment (i.e. PCHEs and electrical equipment). How important are the identified phenomena to predict the thermal and aerosols insult to nearby equipment, and with what adequacy can they be modeled?

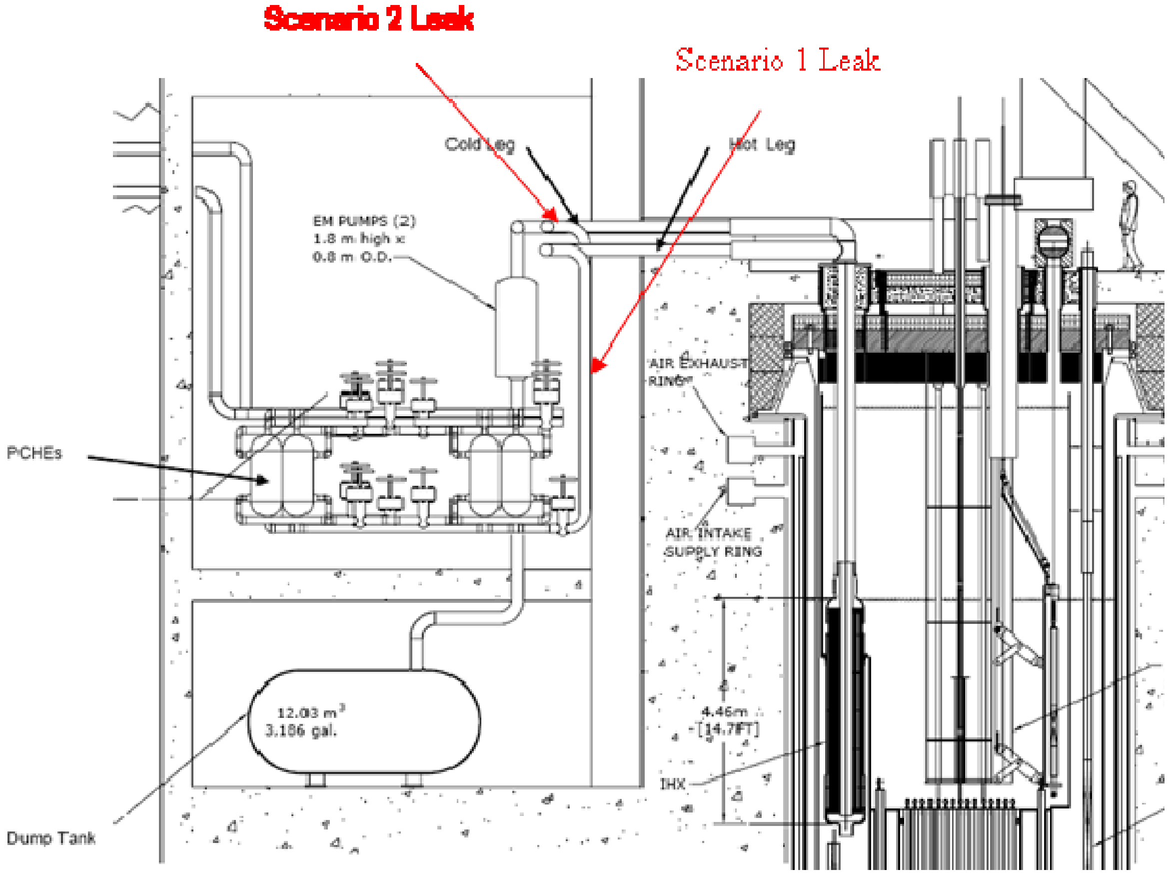

Figure 3-1: The IHTS System [1]

3.2 Details of Scenario 2: Sodium Spray Fire in Cold Leg

The second fire scenario is a postulated leak in the cold side of the IHTS, which results in a sodium spray fire. The location of the leak is in a pipe joint in the cold leg of the secondary loop, immediately downstream from an EM pump (shown in Figure 3-1). The properties of the sodium flowing through this pipe are listed below:

Temperature: 326 °C
Density: ~940 kg/m^3
Pressure: 0.2 MPa (gauge)
Pipe Flow Rate: 645 kg/s
Pipe Flow Velocity: 6.5 m/s

A small crack develops at this joint, resulting in a sodium spray fire with a flow rate of 0.2 kg/s. This spray persists for nearly 10 minutes before corrective actions are taken, resulting in approximately 120 kg of sodium being released. As seen in Figure 3-2, the spray region could include the heat exchangers for the power conversion unit. These heat exchangers could be either sodium-to-CO_2 PCHE's or sodium-to-water (steam generators).

The figure of merit for Scenario 2 is the ability to predict the thermal and aerosols insult to nearby equipment (i.e. PCHEs and electrical equipment).

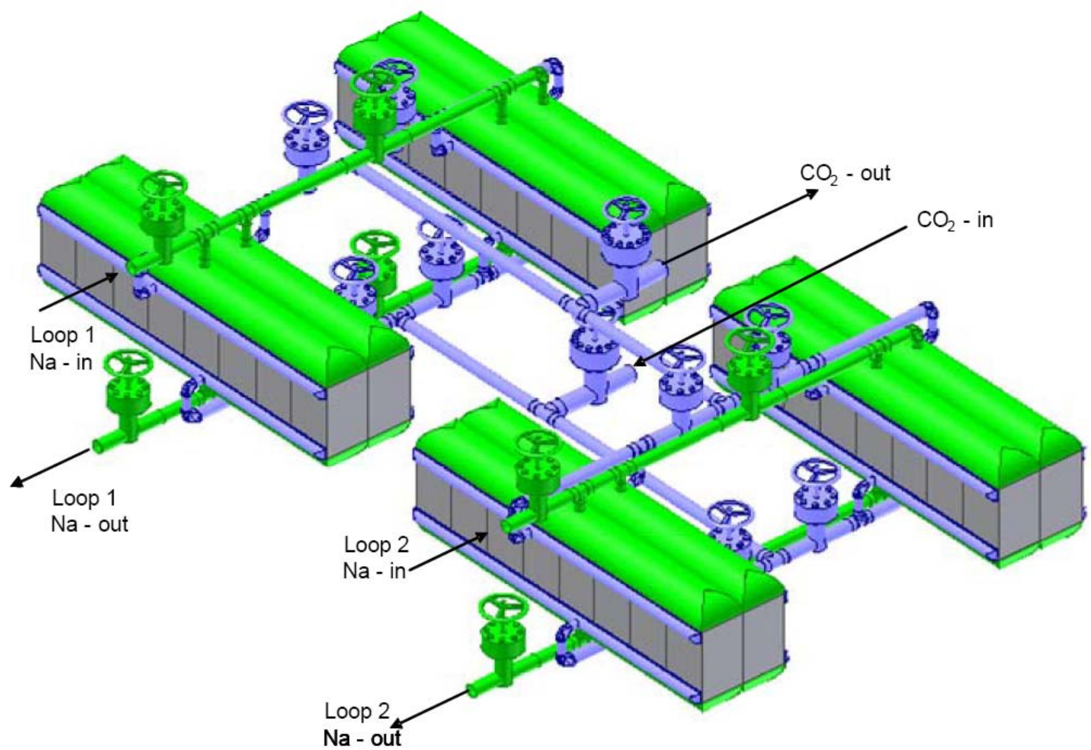

Figure 3-2: Potential Configuration of PCHE's [1].

4 PIRT PHENOMENA

This section will present the results of the PIRT exercise for both scenarios. It should be noted that there was a second cut at the importance rankings for the phenomena that were identified as high importance, because after reviewing the initial table it was apparent that over half the total phenomena were ranked as high importance. Therefore, the second cut was applied to some of the high importance ranking phenomena in order to delineate and make a finer gradation between them. There were some phenomena that were not in the second cut by the panel and their rankings remain high importance based on the previous description. The second cut ranking scheme is as follows:

High3 (H3): of the very highest importance to the figure of merit
High2 (H2): of moderately high importance to the figure of merit
High1 (H1): of less importance than either of the above, but still important to the figure of merit.

The phenomena list that was identified by the panelists for both scenarios is listed below. The number scheme will remain the same for both scenarios. Not all phenomena are applicable to both scenarios.

1. Pool Fire Surface Burning

- A. Radiation Flux from Pool Burning Surface
- B. Radiation Flux to Pool Burning Surface
- C. Mass Burning Rate
- D. Pool Heating Rate
- E. Mass Burning Rate if Radiation is Important
- F. Conduction/Convective Flux
- G. Near Surface Size and Distribution of Aerosol Particles
- H. Damaged State (Complex Surfaces)
- I. Gaseous Products of Metal Reaction and Velocity of Gaseous Products Coming off of the Surface
- J. Source of Sodium Aerosols
- K. Treatment of the Oxide Crust
- L. Film Thickness in Sodium Pool Spreading (Viscosity Issue)
- M. Burning on Surface
- N. Pressure Effect on Combustion (Vapor)

2. Plume Dynamics

- A. Momentum Transport (i.e. Velocity Field)
- B. Turbulence Production
- C. Mixing (Turbulence Model), Oxidizer Transport
- D. Temperature Distribution (Fluctuations)

3. Spray Dynamics

- A. Prediction of Droplet Particle Average Velocity
- B. Prediction of Droplet Particle Velocity Distribution/Range
- C. Prediction of Single Droplet Particle Average Size
- D. Prediction of Droplet Particle Size Distribution/Range

E. Droplet Particle Velocity Variation/Range
F. Particle Clouds over Multiple Control Volumes (Basic Capability)
G. Particle Clouds over Multiple Control Volumes (Effects of Solid Interactions/Flow Strain)
H. Basic Evaporation/Combustion Models
I. Finite-Slip Corrections to Evaporation/Combustion Models
J. Transition to Group Combustion Mode
K. Multi-Component Droplet Capabilities
L. Source for Sodium Aerosols
M. Chemical Kinetics of Sodium Combustion
N. Molecular Diffusion Coefficient Across Diffusion Flame
O. Gas-Band Radiation from Diffusion Flames
P. Radiation from Aerosols in Diffusion Flame
Q. Mass Flux of Aerosols through Diffusion Flame (i.e. diff-diff)
R. Sodium Particle Collision
S. Inertial Impact of Molten Sodium
T. Burning on Surface

4. Aerosol Dynamics

A. Source of Sodium Aerosols
B. Thermopheric Transport of Aerosols
C. Radiation to/from Individual Aerosols
D. Electrical Properties
E. Turbulent Inertial Deposition
F. Gravitational Settling
G. Interception
H. Electro-Static Deposition
I. Aerosol Agglomeration
J. Hydrolysis of Peroxides
K. Aerosol Particle Charging
L. Sodium Carbonate Deposition
M. Sodium Hydroxide Aerosol Deposition
N. Sodium Peroxide Aerosol Deposition
O. Thermal Interaction of Deposit Layer for Aerosol Mixture (i.e. an Effective Conductivity Model or other Treatment)
P. Effective Emissivity of Deposit Layer
Q. Thermophoresis Effect on Deposition Flux

5. Radiation Heat Transfer

A. Radiation to/from Individual Aerosols
B. Radiation Transport for Absorption/Emission
C. Radiation Transport for Scattering
D. Lagrangian Absorption/Emissive Coupling with Radiation Field
E. Spectral Dependence of Radiation Field
F. Lagrangian Scattering Coupling with Radiation Field
G. Overall Joint-Temperature-Absorption Coefficient Distribution
H. Gas-Band Radiation from Diffusion Flames

6. Concrete-Sodium Interactions

   A. Hydrogen Production

7. **Liquid Molten Jet**
   A. Liquid Splashing on Solid
   B. Liquid into Pool
   C. Liquid Jets, Jet Breakup
   D. Vapor Jet into Liquid
   E. Spray Formation in Vapor Jet
8. **Chemistry (Needed for Quenching)**
   A. Burning on Surface
   B. Condensed-Phase Reactions with Substrate
   C. Wetting/Sticking Properties of Sodium on Expected Surfaces

5 PIRT RESULTS AND DISCUSSION

The phenomena identification and ranking tables themselves are the output of the PIRT process. However, as a part of the reporting process, the raw tables have been analyzed and the identified phenomena have been summarized based on four levels of overall importance. The overall importance is judged based on two factors; namely, the importance ranking assigned by the panelists and the state of knowledge ranking. The overall importance levels are defined as follows:

- Level 1: The highest level of overall importance is assigned to those phenomena that were ranked with a *high* level of importance and a *low* state of knowledge.
- Level 2: The second level of overall importance was assigned to those phenomena that were ranked with either a *high* importance and *medium* state of knowledge or *medium* importance and *low* state of knowledge.
- Level 3: The third level was assigned to those phenomena that were given one of the following rankings: high importance with a high state of knowledge; medium importance with either a medium or high state of knowledge; or low importance given with having a low, medium, or high state of knowledge. These rankings reflect a panel opinion that the phenomena are either important but well understood, or are relatively unimportant.
- Level 4: The fourth level of overall importance was assigned to those phenomena that were ranked as uncertain by the panelists for importance ranking and/or state of knowledge rankings. This level represents areas that might require further exploration before a true assessment of importance and state of knowledge is possible.

This section of the report presents the phenomena presented by the overall importance levels described above. These levels were identified in order to delineate research priority for the sodium fire experiments and modeling. The detailed results for each phenomenon can be found in Appendix B.

5.1 Scenario 1, Sodium Pool Fire PIRT Results

This section presents the results of the PIRT specifically for Scenario 1, which is a sodium pool fire. Table 5-1 presents the Level 1 phenomena. Table 5-2 presents the Level 2 phenomena. Table 5-3 through Table 5-7 displays the Level 3 phenomena. Table 5-8 presents the Level 4 Phenomena.

In reviewing Table 5-1, the Level 1 phenomena for Scenario 1 will be discussed. For Pool ***Fire Surface Burning*** there are four sub-phenomena that were analyzed as having Level 1 research priority. The first is *mass burning rate if radiation is important,* which was ranked with a high importance ranking because this phenomena for pool fires will affect the heat release rate. The state of knowledge rankings were low for all categories and it was noted that the uncertainties with this phenomenon are the sodium optical properties. The next sub-phenomena is *near surface size and distribution of aerosol particles*, which was ranked with an importance ranking of Medium to High2 based on the uncertainty associated with the near field distribution.

This uncertainty is reflected in the low state of knowledge rankings. The next sub-phenomenon is *source of sodium aerosols*, which was ranked with High3 importance and low state of knowledge rankings. This refers to the fraction of oxide that is released as aerosol versus the fraction deposited within the pool, the former having consequences for radiative heat transfer and especially for the aerosol exposure of surrounding equipment. In previous work related to sodium combustion there has been little research done for sodium aerosols, and the available data shows substantial scatter. This topic area was a reoccurring theme throughout the PIRT. The final sub-phenomenon for this topic was the *film thickness in sodium pool spreading (viscosity issue)*, which was ranked with an importance ranking from Medium to High3. These rankings were associated with the uncertainty in this phenomenon. The overall state of knowledge rankings for this phenomenon were low.

The next topic for the Level 1 phenomena is ***Aerosol Dynamics***, which has one sub-phenomenon associated with it. This sub-phenomenon is *source of sodium aerosols*, which was ranked with a high importance ranking and a low state of knowledge. Past research does not put an emphasis on this phenomenon.

The ***Concrete-Sodium Interaction*** topic has the sub-phenomenon, *hydrogen production* associated with it. As shown in Table 5-1 this phenomenon was ranked with a high importance ranking with an overall low state of knowledge. This is important in nuclear power plant applications because of the large amounts of concrete in these facilities. There has been research done in the past, the panelists mentioned the uncertainties associated with the large variety of concrete compositions.

The next topic in Table 5-1 is ***Liquid Molten Jet*** with one sub-phenomena associated with it. This sub-phenomenon is *liquid into pool* that refers to the formation of a pool from liquid molten sodium impinging on a surface. It was ranked with a high importance ranking with an overall low state of knowledge. The most significant uncertainties with this phenomenon are with the rate of spreading of the sodium pool and the physics of quenching the sodium pool in regards to the heat transfer balance.

The final topic in Table 5-1 is ***Chemistry***, which also has one sub-phenomenon associated with it. This sub-phenomenon is *condensed-phase reaction with substrate*, which was also analyzed with a Level 1 research priority. The high importance ranking for this phenomenon is based on the potential for sodium-concrete reaction, which will produce hydrogen gas. As indicated above, there is some available data with corresponding phenomenological models, but the applicability of these is unknown given the wide variety of concrete compositions and characteristics.

5.2 Scenario 2, Sodium Spray Fire PIRT Results

This section presents the results of the PIRT specifically for Scenario 2, which is a sodium spray fire. Table 5-9 presents the Level 1 phenomena. Tables 5.10 and 5.11 present the Level 2 phenomena. Tables 5.12 through 5.14 display the Level 3 phenomena. Table 5.15 presents the Level 4 Phenomena.

In reviewing Table 5-9, the Level 1 phenomena for Scenario 2 will be discussed. The first topic is ***Pool Fire Surface Burning***, which has two sub-phenomena associated with the Level 1 research priorities. Both of these phenomena are related to the possible deposition of non-oxidized sodium droplets on surfaces, and the potential for this deposit to burn on the surface. The first sub-phenomena is the *film thickness in sodium pool spreading (viscosity issue),* which was also a Level 1 research priority for Scenario 1. This phenomenon was ranked with an importance ranking from Medium to High3, which was associated with the large uncertainty in the range of scenarios: for a range of leak characteristics the deposit of burning droplets will be sensitive to the spreading (or lack of spreading) of the deposit. The overall state of knowledge rankings for this phenomenon was determined to be low. The next sub-phenomenon is *burning on surface* which is important for a sodium spray fire. The state of knowledge rankings overall were low, in particular because of the uncertainties in the spreading rates and the effect of the oxidation that already occurred in the spray mode. The adequacy of the models and codes were low, but the available input data was medium since some research has been performed.

The next Level 1 topic in Table 5-9 is ***Spray Dynamics***. The first of two sub-phenomena associated with this topic is *source of sodium aerosols,* which was ranked with a high importance and a low state of knowledge. This phenomenon pertains to the fraction of oxides that remain with the droplet versus the fraction that aerosolizes. The second sub-phenomenon is *burning on surface* which has been a recurring theme for the Level 1 research priority for this PIRT. This phenomenon was ranked with a high importance ranking and an overall low state of knowledge.

The next topic is ***Liquid Molten Jet*** with one sub-phenomenon associated with it. This sub-phenomenon is *liquid into pool*, which is specific to the non-oxidized sodium spray, potentially containing larger liquid slugs, collecting on a surface. This is associated with the aforementioned pool fire surface burning issues. It was ranked with a high importance ranking with an overall low state of knowledge. The uncertainties with this phenomenon are based on the difficulties with the heat transfer balance of quenching the pool of sodium that is forming on the surface.

The final topic in Table 5-9 is ***Chemistry (Needed for Quenching)***, which has two sub-phenomena associated with it. The first sub-phenomenon is *burning on surface,* which was specific to the sodium hitting an object and burning. This phenomenon was ranked with a high importance and an overall low state of knowledge. The second sub-phenomenon is *condensed-phase reaction with substrate*, which was also analyzed with a Level 1 research priority. The high importance ranking for this phenomenon was based on the potential for sodium-concrete reaction, which will produce hydrogen gas.

5.3 Summary of Research Priority Phenomena

This section will present a summary of the general research priorities obtained through the PIRT process for both scenarios. The focus for this section is on the research priorities that will be further researched throughout this program. The general topics include aerosol dynamics and surface burning, radiative heat transfer, and sodium chemistry related to quenching.

5.3.1 Oxides aerosol, crust, or solution

Sodium can oxidize on its surface, but tends towards steady-state oxidation in the gas phase. Oxides of sodium can form aerosols, particularly if the oxidation occurs in the gas phase, but it has been observed that only a fraction of the oxide produced forms an aerosol with the fraction of aerosol reported ranging from 0.1 to 0.7. The remaining oxide forms either a crust on the surface of the sodium metal or ends up within the metal (either as a solution or precipitate). Previous work has discussed the evolution of surface oxide crusts to solutions or precipitates as a function of the pool temperature. The fraction that forms an aerosol is important for two reasons: this oxide is removed from the crust (next paragraph) and the consequences of the aerosolized oxide, being a significant hazard to electrical equipment, can extend much farther.

5.3.2 Surface burning and oxygen transport through oxide crusts

Sodium oxidation is generally observed to be limited by oxygen transport (models based on this concept have performed well in the past). However, existing correlations of burning rates are for pools at steady-state temperatures on the order of 1000 K where oxides melt and sink to the bottom of pools. At lower temperatures relevant to suppression and consequence mitigation, oxides form a porous crust on the surface that may inhibit oxidizer transport and thereby the rate of heat release associated with pools. Since substantial thermal damage is hypothesized to occur in close vicinity to sodium pool fires the prediction of the oxidation rate will be important for predicting thermal damage to surfaces on which sodium pools form.

5.3.3 Radiative heat transfer

Oxidizing sodium can lose a substantial thermal energy through radiative transport. This radiative transport takes thermal energy away from the sodium that deposits on surfaces and can put that thermal load on nearby equipment. We are unaware of heat transfer measurements in sodium pool fires that measure this radiative heat transfer, and propose to carry out appropriate measurements. These measurements are carried out using heat flux gauges around spray and pool fires.

5.3.4 Thermal coupling of sodium pools to surfaces

The high thermal conductivity of sodium that makes it desirable as a reactor coolant also leads to rapid heat transfer between sodium that pools on surfaces following sprays and pours. Initial analysis carried out by our group suggests that, until the facility surfaces reach the sodium temperatures, the fastest heat transfer will often be through thermal coupling (conduction) of sodium pools to surfaces. For example, the thermal conductivity time scale (thickness^2/thermal diffusivity) for sodium for a centimeter thick layer is less than one second. This is much less than the oxidation time for pool burning so that we can expect pool fires for many spills to be occurring at temperatures close to the surface temperatures where the sodium pools. We are not aware of any measurements of the thermal insult to surfaces below sodium pools. These measurements are also useful for characterizing pool oxidation rates when the majority of the heat release is transmitted through the pool to the surface below.

Table 5-1: Level 1 Phenomena for Scenario 1, Sodium Pool Fire

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 1: Pool Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
1. Pool Fire Surface Burning							
E. Mass Burning Rate if Radiation is Important	H1	L	L	L	L	L	L
G. Near Surface Size and Distribution of Aerosol Particles	H2 to M	L	L	L	L	L	L
J. Source of Sodium Aerosols	H3	L	L	L	L	L	L
L. Film Thickness in Sodium Pool Spreading (Viscosity Issue)	H3 to M	M	L	L	M	L	L
4. Aerosol Dynamics							
A. Source of Sodium Aerosols	H	L	L	L	L	L	L
6. Concrete-Sodium Interactions							
A. Hydrogen Production	H	M	L	L	M	L	L
7. Liquid Molten Jet							
B. Liquid into Pool	H	L	L	L	H	L	M
8. Chemistry (Needed for Quenching)							
B. Condensed-Phase Reactions with Substrate	H	M	L	L	L	L	L

Table 5-2: Level 2 Phenomena for Scenario 1, Sodium Pool Fire

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 1: Pool Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
1. Pool Fire Surface Burning							
C. Mass Burning Rate	H3	M	L	M	H	M	M
D. Pool Heating Rate	H2	M	L	M	H	M	M
4. Aerosol Dynamics							
B. Thermopheric Transport of Aerosols	H	M	M	L	M	L	M
D. Electrical Properties	H	M	M	L	M	L	M
L. Sodium Carbonate Deposition	H	M	M	M	M	M	M
M. Sodium Hydroxide Aerosol Deposition	H	M	M	M	M	M	M
N. Sodium Peroxide Aerosol Deposition	H	M	M	M	M	M	M
Q. Thermophoresis Effect on Deposition Flux	H	M	M	L	M	L	M
5. Radiation Heat Transfer							
G. Overall Joint-Temperature-Absorption Coefficient Distribution	M	M	L	L	L	L	L
7. Liquid Molten Jet							
A. Liquid Splashing on Solid	H	M	L	M	M	M	M

Table 5-3: Level 3 Phenomena for Scenario 1, Sodium Pool Fire (1 of 5)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 1: Pool Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
1. Pool Fire Surface Burning							
A. Radiation Flux from Pool Burning Surface	L	X*	X	X	X	X	X
B. Radiation Flux to Pool Burning Surface	L	X	X	X	X	X	X
F. Conduction/Convective Flux	H2	H	H	H	NA†	L	L
I. Gaseous Products of Metal Reaction and Velocity of Gaseous Products Coming off of the Surface	L						
K. Treatment of the Oxide Crust	L	X	X	X	X	X	X
M. Burning on Surface	L	L	L	M	M	L	L
N. Pressure Effect on Combustion (Vapor)	L	X	X	X	X	X	X
2. Plume Dynamics		X	X	X	X	X	X
A. Momentum Transport (i.e. Velocity Field)	H	H	H	H	NA	H	NA
B. Turbulence Production	M	H	H	M	M	H	NA
C. Mixing (Turbulence Model), Oxidizer Transport	H	H	H	H	NA	H	NA
D. Temperature Distribution (Fluctuations)	M	H	H	M	M	H	NA

* The “X” in the tables represents where the panel did not provide input.
† The “NA” stands for Not Applicable.

Table 5-4: Level 3 Phenomena for Scenario 1, Sodium Pool Fire (2 of 5)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 1: Pool Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
3. Spray Dynamics							
A. Prediction of Droplet Particle Average Velocity	L	H	H	H	NA	H	NA
B. Prediction of Droplet Particle Velocity Distribution/Range	L						
C. Prediction of Single Droplet Particle Average Size	L	M	M	L	L	L	L
D. Prediction of Droplet Particle Size Distribution/Range	L	M	M	L	L	L	L
E. Droplet Particle Velocity Variation/Range	L	M	M	L	L	L	L
F. Particle Clouds over Multiple Control Volumes (Basic Capability)	L	X	X	X	X	X	X
G. Particle Clouds over Multiple Control Volumes (Effects of Solid Interactions/Flow Strain)	L	X	X	X	X	X	X

Table 5-5: Level 3 Phenomena for Scenario 1, Sodium Pool Fire (3 of 5)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 1: Pool Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
3. Spray Dynamics (Cont.)							
H. Basic Evaporation/Combustion Models	L	H	H	M	NA	H	NA
I. Finite-Slip Corrections to Evaporation/Combustion Models	L	H	H	H	H	H	H
J. Transition to Group Combustion Mode	L	X	X	X	X	X	X
K. Multi-Component Droplet Capabilities	L	X	X	X	X	X	X
L. Source for Sodium Aerosols	L	L	L	L	L	L	L
M. Chemical Kinetics of Sodium Combustion	L	X	X	X	X	X	X
N. Molecular Diffusion Coefficient Across Diffusion Flame	L	H	H	H	NA	M	L
O. Gas-Band Radiation from Diffusion Flames	L	X	X	X	X	X	X
P. Radiation from Aerosols in Diffusion Flame	L	L	L	L	L	L	L
Q. Mass Flux of Aerosols through Diffusion Flame (i.e. diff-diff)	L	L	L	L	L	L	L

Table 5-6: Level 3 Phenomena for Scenario 1, Sodium Pool Fire (4 of 5)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 1: Pool Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
3. Spray Dynamics (Cont.)							
R. Sodium Particle Collision	L	X	X	X	X	X	X
S. Inertial Impact of Molten Sodium	L	M	L	M	L	M	L
T. Burning on Surface	L	L	L	M	M	L	L
4. Aerosol Dynamics							
F. Gravitational Settling	H	H	H	M	H	M	H
I. Aerosol Agglomeration	H	H	H	M	M	M	M
O. Thermal Interaction of Deposit Layer for Aerosol Mixture (*i.e.* an Effective Conductivity Model or other Treatment)	L	X	X	X	X	X	X
P. Effective Emissivity of Deposit Layer	L	X	X	X	X	X	X

Table 5-7: Level 3 Phenomena for Scenario 1, Sodium Pool Fire (5 of 5)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 1: Pool Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
5. Radiation Heat Transfer							
B. Radiation Transport for Absorption/Emission	H	H	H	M	M	H	NA
C. Radiation Transport for Scattering	H	H	H	L	M	H	NA
D. Lagrangian Absorption/Emissive Coupling with Radiation Field	L	H	L	NA	NA	NA	NA
F. Lagrangian Scattering Coupling with Radiation Field	L	H	L	L	M	H	NA
H. Gas-Band Radiation from Diffusion Flames	L	X	X	X	X	X	X
7. Liquid Molten Jet							
C. Liquid Jets, Jet Breakup	L	M	M	H	NA	H	NA
D. Vapor Jet into Liquid	L	X	X	X	X	X	X
E. Spray Formation in Vapor Jet	L	X	X	X	X	X	X
8. Chemistry (Needed for Quenching)							
A. Burning on Surface	L	L	L	M	M	L	L

Table 5-8: Level 4 Phenomena for Scenario 1, Sodium Pool Fire

Phenomenon	Importance Rankings		State of Knowledge Rankings					
	Scenario 1: Pool Fire		Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
1. Pool Fire Surface Burning								
H. Damaged State (Complex Surfaces)	H3-H1		X	X	X	X	X	X
4. Aerosol Dynamics								
C. Radiation to/from Individual Aerosols	M		X	X	X	X	X	X
E. Turbulent Inertial Deposition	M		X	X	X	X	X	X
G. Interception	M		X	X	X	X	X	X
H. Electro-Static Deposition	M		X	X	X	X	X	X
J. Hydrolysis of Peroxides	M		X	X	X	X	X	X
K. Aerosol Particle Charging	U		X	X	X	X	X	X
5. Radiation Heat Transfer								
A. Radiation to/from Individual Aerosols	M		X	X	X	X	X	X
E. Spectral Dependence of Radiation Field	U		H	L	L	M	H	NA
8. Chemistry (Needed for Quenching)								
C. Wetting/Sticking Properties of Sodium on Expected Surfaces	H		M	L	U	U	U	U

Table 5-9: Level 1 Phenomena for Scenario 2, Sodium Spray Fire

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 2, Spray Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
1. Pool Fire Surface Burning							
L. Film Thickness in Sodium Pool Spreading (Viscosity Issue)	H	M	L	L	M	L	L
M. Burning on Surface	H	L	L	M	M	L	L
3. Spray Dynamics							
L. Source for Sodium Aerosols	H	L	L	L	L	L	L
T. Burning on Surface	H	L	L	M	M	L	L
7. Liquid Molten Jet							
B. Liquid into Pool	H	L	L	L	H	L	M
8. Chemistry (Needed for Quenching)							
A. Burning on Surface	H	L	L	M	M	L	L
B. Condensed-Phase Reactions with Substrate	H	M	L	L	L	L	L

Table 5-10: Level 2 Phenomena for Scenario 2, Sodium Spray Fire (1 of 2)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 2, Spray Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
Plume Dynamics							
Turbulence Production	M	H	H	M	M	H	NA
Temperature Distribution (Fluctuations)	M	H	H	M	M	H	NA
3. Spray Dynamics							
C. Prediction of Single Droplet Particle Average Size	H	M	M	L	L	L	L
P. Radiation from Aerosols in Diffusion Flame	M	L	L	L	L	L	L
Q. Mass Flux of Aerosols through Diffusion Flame (i.e. diff-diff)	M	L	L	L	L	L	L
S. Inertial Impact of Molten Sodium	M	M	L	M	L	M	L
4. Aerosol Dynamics							
B. Thermopheric Transport of Aerosols	H	M	M	L	M	L	M
D. Electrical Properties	H	M	M	L	M	L	M
L. Sodium Carbonate Deposition	H	M	M	M	M	M	M
M. Sodium Hydroxide Aerosol Deposition	H	M	M	M	M	M	M
N. Sodium Peroxide Aerosol Deposition	H	M	M	M	M	M	M
Q. Thermophoresis Effect on Deposition Flux	H	M	M	L	M	L	M

Table 5-11: Level 2 Phenomena for Scenario 2, Sodium Spray Fire (2 of 2)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 2, Spray Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
5. Radiation Heat Transfer							
D. Lagrangian Absorption/Emissive Coupling with Radiation Field	H	H	L	NA	NA	NA	NA
F. Lagrangian Scattering Coupling with Radiation Field	H	H	L	L	M	H	NA
6. Concrete-Sodium Interactions							
A. Hydrogen Production	H	M	L	L	M	L	L
7. Liquid Molten Jet							
A. Liquid Splashing on Solid	H	M	L	M	M	M	M
C. Liquid Jets, Jet Breakup	H	M	M	H	NA	H	NA
8. Chemistry (Needed for Quenching)							
C. Wetting/Sticking Properties of Sodium on Expected Surfaces	H	M	L	U	U	U	U

Table 5-12: Level 3 Phenomena for Scenario 2, Sodium Spray Fire (1 of 3)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 2, Spray Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
1. Pool Fire Surface Burning							
A. Radiation Flux from Pool Burning Surface	L	X	X	X	X	X	X
B. Radiation Flux to Pool Burning Surface	L	X	X	X	X	X	X
C. Mass Burning Rate	L	M	L	M	H	M	M
D. Pool Heating Rate	L	M	L	M	H	M	M
E. Mass Burning Rate if Radiation is Important	L	L	L	L	L	L	L
F. Conduction/Convective Flux	L	H	H	H	NA	L	L
H. Damaged State (Complex Surfaces)	L	X	X	X	X	X	X
I. Gaseous Products of Metal Reaction and Velocity of Gaseous Products Coming off of the Surface	L	X	X	X	X	X	X
K. Treatment of the Oxide Crust	L	X	X	X	X	X	X
N. Pressure Effect on Combustion (Vapor)	L	X	X	X	X	X	X
2. Plume Dynamics							
A. Momentum Transport (i.e. Velocity Field)	H	H	H	H	NA	H	NA
C. Mixing (Turbulence Model), Oxidizer Transport	H	H	H	H	NA	H	NA

Table 5-13: Level 3 Phenomena for Scenario 2, Sodium Spray Fire (2 of 3)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 2, Spray Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
3. Spray Dynamics							
A. Prediction of Droplet Particle Average Velocity	H	H	H	H	NA	H	NA
B. Prediction of Droplet Particle Velocity Distribution/Range	L	X	X	X	X	X	X
D. Prediction of Droplet Particle Size Distribution/Range	M	M	M	L	L	L	L
E. Droplet Particle Velocity Variation/Range	M	M	M	L	L	L	L
F. Particle Clouds over Multiple Control Volumes (Basic Capability)	L	X	X	X	X	X	X
G. Particle Clouds over Multiple Control Volumes (Effects of Solid Interactions/Flow Strain)	L	X	X	X	X	X	X
H. Basic Evaporation/Combustion Models	H	H	H	M	NA	H	NA
I. Finite-Slip Corrections to Evaporation/Combustion Models	M	H	H	H	H	H	H
J. Transition to Group Combustion Mode	L	X	X	X	X	X	X
K. Multi-Component Droplet Capabilities	L	X	X	X	X	X	X
M. Chemical Kinetics of Sodium Combustion	L	X	X	X	X	X	X

Table 5-14: Level 3 Phenomena for Scenario 2, Sodium Spray Fire (3 of 3)

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 2, Spray Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
3. Spray Dynamics (Cont.)							
N. Molecular Diffusion Coefficient Across Diffusion Flame	H	H	H	H	NA	M	L
O. Gas-Band Radiation from Diffusion Flames	L	X	X	X	X	X	X
R. Sodium Particle Collision	L	X	X	X	X	X	X
4. Aerosol Dynamics							
F. Gravitational Settling	H	H	H	M	H	M	H
I. Aerosol Agglomeration	H	H	H	M	M	M	M
O. Thermal Interaction of Deposit Layer for Aerosol Mixture (*i.e.* an Effective Conductivity Model or other Treatment)	L						
P. Effective Emissivity of Deposit Layer	L	X	X	X	X	X	X
5. Radiation Heat Transfer							
B. Radiation Transport for Absorption/Emission	H	H	H	M	M	H	NA
C. Radiation Transport for Scattering	H	H	M	L	M	H	NA
G. Overall Joint-Temperature-Absorption Coefficient Distribution	M	M	L	L	L	L	L
H. Gas-Band Radiation from Diffusion Flames	L	X	X	X	X	X	X
7. Liquid Molten Jet							
D. Vapor Jet into Liquid	L	X	X	X	X	X	X

Table 5-15: Level 4 Phenomena for Scenario 2, Sodium Spray Fire

Phenomenon	Importance Rankings	State of Knowledge Rankings					
	Scenario 2, Spray Fire	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data
4. Aerosol Dynamics							
C. Radiation to/from Individual Aerosols	M	X	X	X	X	X	X
E. Turbulent Inertial Deposition	M	X	X	X	X	X	X
G. Interception	M	X	X	X	X	X	X
H. Electro-Static Deposition	M	X	X	X	X	X	X
J. Hydrolysis of Peroxides	M	X	X	X	X	X	X
K. Aerosol Particle Charging	U	X	X	X	X	X	X
5. Radiation Heat Transfer							
A. Radiation to/from Individual Aerosols	M	X	X	X	X	X	X
E. Spectral Dependence of Radiation Field	U	H	L	L	M	H	NA

6 PROJECTED EXPERIMENTAL AND MODELING PROGRAM

6.1 Initial Fire Modeling

Fire from sodium leaks can be categorized into the canonical forms of spray fires or pool fires. Spray fires result when droplets burn up appreciably before they fall on surfaces, and pool fires result when the bulk of the sodium forms a pool on the surface prior to oxidizing. The primary factor that determines which of these fires results is the degree of reaction prior to pooling on a surface, if pooling even occurs. The degree of reaction prior to falling onto a surface will depend on the initial droplet sizes and, to a lesser degree, the initial velocities. Other factors include how much the sodium is spread out prior to falling on a surface since excessive dispersion could result in a collection of particles quenched on surfaces. In experiments to simulate accidents, nozzles will be employed to generate an initial distribution of droplets to either burn as a spray or fall to a surface and burn as a pool. For the purpose of designing experiments, we have carried out preliminary sodium spray-fire simulations. The objective is to develop an approximate understanding of the degree of reaction in the spray mode (versus pool mode) that will occur for varying droplet sizes. In this section, some scoping simulations will be described that have been carried out to estimate the degree of oxidation of the sodium in the spray mode for different initial droplet size distributions.

6.1.1 Inputs and assumptions for the sodium spray fire model

These initial calculations were performed using an existing code (Vulcan) at Sandia. Vulcan is a computational fluid dynamics (CFD) code that solves the Reynolds-averaged Navier-Stokes equations including a k-ε model for turbulence to predict the evolution of the gas phase. Sodium particles evolve simultaneously using a Lagrangian approach [2-4]. Sodium oxidation is carried out using a conserved-scalar approach to predict the subgrid transport of heat and oxidizer around the burning droplets; this model includes particle transient heating due to reactions and also radiative cooling [5]. When a spray forms, the initial droplet size is generally a function of the Weber number (the ratio of the kinetic energy to the surface energy), and for sodium, typical droplet sizes are on the order of millimeters. For the present design simulations, we considered the effects of mean droplet sizes of 3mm, 1mm, and 0.5 mm. Generally, a distribution of droplet sizes occurs, and for the present purposes the distribution was presumed to be lognormal with a variance of 0.15 orders of magnitude. Simulations were carried out in a simplified volume geometry (100 m3) and general form (rectangular prism with dimensions 3.33 m x 3.33 m x 9 m high) similar to the Surtsey vessel (described in the subsequent section) where experiments will be carried out. In this volume, there is sufficient oxidizer for approximately 25 kg of sodium to fully oxidize, so simulations were carried out with that mass injected at 1 kg/s. A solid cone spray angle of 20 degrees was also presumed, and particles were injected at 8 m above the vessel floor. Initial particle temperatures are taken to be 500 K, approximately the temperature of a reactor secondary cooling stream. While convective and radiative heat transfer to the walls occurs, the walls are presumed to be thermally massive and thus isothermal. The sodium is assumed to fully oxidize to sodium peroxide (Na2O2), but in the latter parts of these simulations, oxygen depletion is likely sufficient to cause partial oxidation to sodium oxide

(Na_2O); this would over-predict heat release and oxygen consumption late in the simulated evolution. The sodium particles participate radiatively, but the radiative properties for the sodium peroxide aerosol were not included so that the oxide aerosol does not participate; this would tend to over predict radiative transport away from the spray since the oxide should absorb some of the radiant flux.

6.1.2 Results of initial sodium spray fire modeling

Based on these modeling simplifications, simulations were carried out for the three mean droplet sizes (3mm, 1mm, and 0.5 mm) to develop an understanding of the degree of reaction that could be expected in the spray mode. While the CFD approach offers detailed spatial resolution, only global results are presented here. Overall, results showed that the range of droplet sizes considered spans the range from where the spray-fire mode dominates (smaller droplets) to where a pool-fire mode will dominate (the pool fire evolution was not simulated here). This is demonstrated in Figures 6-1 and 6-2 where the distribution of the total mass deposited on surfaces (for pool burning) in Figure 6-1 is contrasted with the total mass oxidized in the spray in Figure 6-2. The three red lines in these figures represent the mass injected for the three different simulations. For the 3 mm droplets, the majority of the sodium is deposited on surfaces and only 15-20% of the mass is oxidized. Sodium oxidation roughly follows the so-called d2-burning-rate law where the burning time is proportional to the initial droplet area, so smaller droplets burn substantially faster. With a mean size of 1 mm, roughly half (44%) of the sodium is oxidized in the spray mode, and with a mean size of 0.5 mm roughly three-quarters (72%) of the sodium is oxidized in the spray mode. (Given the limited current degree of validation, substantial uncertainties should be ascribed to predictions.) Heat release in the spray mode is fast compared to that in pool-fire mode, and the temperature rise and pressure rise can both be substantial in this mode. Predicted temperatures rose to the 1500 K range and pressures approached 20 atmospheres assuming a well-sealed vessel. Oxygen depletion is also significant for the 0.5 mm droplets, and it is clear that sodium oxide rather than sodium peroxide would form during part of the spray combustion. This suggests that the temperatures and pressures indicated above may be over-predicted and future predictions will account for the differences in degree of oxidation appropriate for the different oxygen levels.

The current simulations have not been carried through the pool burning stage because of the importance of the thermal coupling between the deposited sodium and the vessel surfaces. The thermal density of steel is substantial compared to that of sodium (about eight times greater where the thermal density is the product of the density and the specific heat), and the thermal conductivities are high so the sodium is expected to cool upon contact with the vessel floor. This degree of coupling is not currently tied to the full CFD code, but will be employed in subsequent simulations.

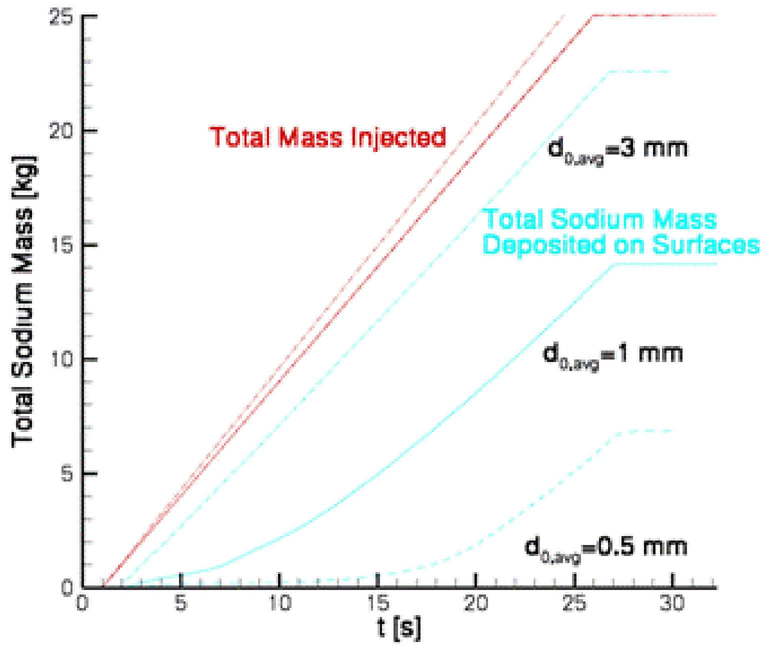

Figure 6-1: Total sodium mass deposited on surfaces

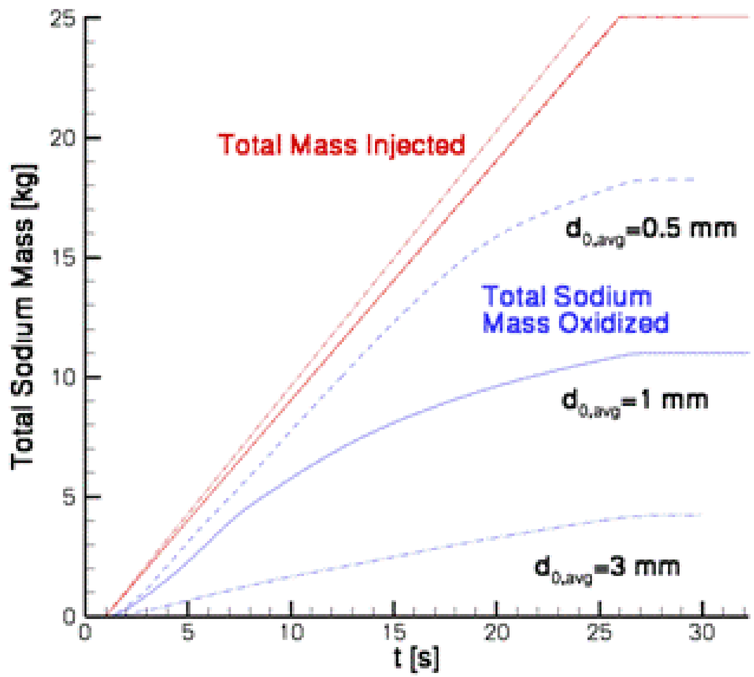

Figure 6-2: Total sodium mass oxidized

6.2 Overview of Experimental Design and Setup

The design and setup for the liquid sodium spray and pool fire experimental program is currently taking place at Sandia. The Surtsey vessel was chosen as the test vessel following a search of available pressure vessels at Sandia. This vessel was designed and used for similar combustion experiments (high-pressure thermite melt ejection, direct containment heating, hydrogen combustion, etc.) and is well-fitted for the experiments.

The Surtsey vessel is an ASME-approved steel pressure vessel. It has a cylindrical shape with removable, dished heads attached to both ends, and is 3.6 m in diameter by 10.3 m high. The Surtsey vessel has a maximum allowable working pressure of 1 MPa at 533 K, but has a burst diaphragm installed to limit the pressure in the vessel to less than 0.9 MPa.

The first sodium experiments are going to be scoping tests with small amounts of sodium (up to 7.5 kg). The objectives of these initial experiments are to:

1. investigate quenching a sodium spill with the stainless steel substrate,
2. demonstrate the conversion of the sodium combustion products to sodium bi-carbonate with the introduction of carbon dioxide gas,
3. understand the performance of the sodium spray nozzles,
4. and gain experience performing small-scale liquid metal experiments with the melt generator system that will be used for the full-scale experiments.

The results of the initial outdoor scoping tests and additional computational analysis will be used to further develop the full-scale in-vessel experiments.

The continuing experimental and model development will focus on sodium spray and pool fires. The data collected from these experiments will be used to develop sodium fire models. A continued review of advanced reactor designs will take place. With this, a pilot safety analysis for one advanced reactor design and one advanced fuel cycle facility design will be performed. Also, guidance for mitigation techniques will be suggested based on the experimental data and modeling results.

7 WORK CITED

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8 DISTRIBUTION

2	MS9018	Central Technical Files	8944
2	MS0899	Technical Library	4536
1	MS0123	D. Chavez, LDRD Office	1011

APPENDIX A: RESUMES OF PIRT PARTICIPANTS

This appendix presents the resumes of the PIRT participants.

THOMAS KEVIN BLANCHAT

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EDUCATION

Ph.D., 1991, Nuclear Engineering, Texas A&M University

M.S., 1988, Nuclear Engineering, Texas A&M University

B.S., 1987, Nuclear Engineering, Texas A&M University.

U.S. Navy 1974-1983, Electronics Technician, Nuclear Reactor Operator, Submarine Service.

FIELDS OF SPECIALIZATION

Nuclear reactor systems and systems modeling, computational and experimental fluid mechanics and heat transfer, two-phase fluid flow visualization using optical imaging techniques, severe accident testing, large-scale hydrocarbon fire experiment programs.

EXPERIENCE

Principal Member Technical Staff, 2002-present, Fire Science & Technology Department, Sandia National Laboratories. Directs SNL experimental programs to develop validation data of the soot and gas species from a quiescent hydrocarbon pool fire and the heat flux incident to an object located within the fire plume for the validation of SNL fire codes. Directs SNL hydrocarbon fuel fire experimental research programs for DoD and DOE customers. Program manager for SNL fire analysis of the Nuclear Regulatory Commission Nuclear Power Plant IVA Project, activities include direction to staff regarding research, computations, and experiments to address vital national security issues. Coordinates all activities at the remote Burn Site test facility and the recently constructed Thermal Test Complex. Currently managing a team of approximately 10 individuals (SNL technologists and contractors).

Principal Member Technical Staff, 1999-2002, Nuclear Safety Testing Department, Sandia National Laboratories; Project Manager for the design, construction, and operation of the In-ground Storage Vault (IGSV) for the Sandia Pulsed Reactor (SPR) fuel materials. Principal Investigator (PI) responsible for design and supervision of all experimental activities relating to the Integral Heat Flux to Objects in Pool Fires, a MAVEN effort involving ASCI code validation. PI responsible for completion and documentation of the SNL Enclosure and China Lake mock B52 bomb bay fire tests.

Senior Member Technical Staff, 1992-1999, Severe Accident Phenomenology Department and Reactor Safety Experiments Department, Sandia National Laboratories; lead experimenter at the Surtsey Test Facility and the Containment Technology Test Facility; scaled experiments are performed at the two test facilities for the U.S. Nuclear Regulatory Commission that simulate hypothetical severe accidents in a nuclear power plant.

Publications:

T. Blanchat, A. Brown, V. Figueroa, S. Yoon, “Benchmark Enclosure Fire Suppression Experiments and Modeling , Suppression and Detection Research and Applications – A Technical Working Conference (SUPDET 2008), Orlando, FL, March 11-13, 2008.

T. Blanchat and V. Figueroa, “Large-Scale Open Pool Experimental Data and Analysis for Fire Model Validation and Development,” accepted to the 9th International Symposium on Fire Safety Science, Karlsruhe, Germany, September 21-26, 2008.

D. Dobranich and T. Blanchat, “Large-Scale Testing and High-Fidelity Simulation Capabilities at Sandia National Laboratories to Support Space Power and Propulsion,” Space Technology and Applications International Forum (STAIF-2008), Albuquerque, NM, February 10-14, 2008.

T. Blanchat, T. O’Hern, S. Kearney, A. Ricks, and D. Jernigan, “Validation Experiments to Determine Radiation Partitioning of Heat Flux to an Object in a Fully Turbulent Fire,” Accepted to the 32nd Symposium (International) on Combustion, Montreal, Canada, August 3-8, 2008.

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Allen, M. D., T. K. Blanchat, M. M. Pilch and R. T. Nichols, 1993, Experiments to investigate the effects of fuel/coolant interactions on direct containment heating: the IET-8A and IET-8B experiments, *SAND92-2849*.

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Blanchat, Thomas K., Sundberg, David W., Brown, Alexander L., 2006, "Well-characterized open pool experiment data and analysis for model validation and development," *SAND2006-7508.*

Blanchat, Thomas K., Nichols, Robert T., 2006, "Experiment report for burning liquid fuel spread in a multi-level structure," Sandia National Laboratories, Albuquerque, NM, *SAND2006-4433*

Blanchat, Thomas K., Sundberg, Wayne D., Brown, Alexander L., 2006, "The long-term environment and thermal response of a representative structure induced by jet fuel fires from scenario-specific events," Sandia National Laboratories, Albuquerque, NM, *SAND2006-2530.*

Ricks, Allen, Blanchat, Thomas K., Jernigan, Dann A., 2006, “Validation experiments to determine radiation partitioning of heat flux to an object in a fully turbulent fire,” Sandia National Laboratories, Albuquerque, NM, *SAND2006-3494.*

John E. Brockmann
Curriculum [redacted] and Publication List

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WORK EXPERIENCE

10/93 - Present
Aerosol Scientist, Engineering Sciences Center, Sandia National Laboratories.

- Testing and modeling of aerosol based application of decontamination material to surfaces
- Source term measurement for spent reactor fuel sabotage program
- Interior aerosol transport experiments and modeling for chem-bio threats
- Sampling method development for chem-bio threats
- Source term testing and modeling for improvised dispersion devices for chem-bio-rad/nuc threats
- Source term experiments for high energy disruption of spent nuclear fuel elements
- Soot modeling for fire research
- Particle focusing research for cold spray processing
- Technical support to DOE for Pantex EIS: aerosol deposition and source modeling
- Phase Doppler Particle Analyzer (PDPA) measurements of particle size and velocity in thermal sprays.
- Gas phase nucleation modeling in Chemical Vapor Deposition (CVD) reactors
- Particle contamination in semiconductor manufacturing
- Contamination Free Manufacturing (CFM)
- Aerosol sampling DOE consultant on filtration

3/81 - 10/93
Aerosol Scientist, Severe Accident Phenomenology Department, Sandia National Laboratories.

- Aerosol source term investigation in Nuclear Reactor Accidents
- Aerosol sampling and measurement
- Aerosol equipment design and calibration
- Aerosol behavior modeling Consultant to DOE's Advisory Committee on Nuclear Facility Safety
- Space Nuclear Thermal Propulsion
- Gas treatment and cleaning
- Expert panel on Dispersion and Deposition Uncertainty Assessment for Joint USNRC/ CEC Probabilistic Accident Consequence Uncertainty Analysis

FORMAL EDUCATION

- Ph.D., Mechanical Engineering, University of Minnesota, 1981
- M.A., Economics, University of Minnesota, 1977
- M.S.M.E.,Mechanical Engineering, University of Minnesota, 1976
- B.M.E., Mechanical Engineering, University of Minnesota, 1974

OTHER AREAS OF EXPERTISE

- Aerosol sampling and transport
- Aerosol measurement
- Aerosol dynamics and behavior

OTHER SKILLS/EXPERIENCE/ACTIVITIES NOT LISTED ABOVE

- American Association for Aerosol Research (AAAR) Board of Directors, 6 years
- AAAR Secretary (1999-2001)
- AAAR Secretary-Elect (1998-1999)
- AAAR By-Laws Committee Chair, 2 years
- AAAR Nuclear and Radioactive Aerosols Working Group Chair, 3 years

PATENTS

- 6,348,687 (Aerodynamic beam generator for large particles)
- 6,386,015 (Apparatus to collect, classify, concentrate, and characterize gas-borne particles)
- 6,664,550 (Apparatus to collect, classify, concentrate, and characterize gas-borne particles)
- 5,793,478 (Apparatus for measuring particle properties)

Sandia National Laboratories EMPLOYEE RECOGNITION AWARDS

- 2007: Access Delay Development Team
- 2003: Sandia Bio Defense Initiative Test bed Team
- 2001: PROTECT Chem-Bio Demonstration Team
- 1998: 911-Bio ACTD Analysis Team

SELECTED PUBLICATIONS

Book Chapters

Brockmann, J.E. (2001) "Sampling and Transport of Aerosols," Chapter 8 in Aerosol Measurement, P.A. Baron and K. Willeke, eds., John Wiley and Sons, New York.

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Tarbell, WW; Brockmann, JE; Washington, KE; Pilch, M.; Marx, KD (1988) “Direct containment heating and aerosol generation during high-pressure-melt expulsion experiments,” Transactions of the American Nuclear Society, vol.57, p.361

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Brockmann, J. E., McMurry, P. H., and Lui, B. Y. H. (1982) “On Simultaneous Coagulation and Diffusional Loss of Free-Molecule Aerosols in Turbulent Pipe Flow,” Aerosol Science and Technology, v.1, no.2, p.163-178

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T.Y. Chu received his B.S. from Purdue University, and MS and PhD from the University of Minnesota, all in Mechanical Engineering. He is a Senior Scientist at Sandia, which is the highest technical position at Sandia National Laboratories. It is a "Special Appointment" position in recognition of sustained high performance and the ability to provide strategic vision and direction to major Laboratory programs. Over his 37-year career, he has made contributions to a wide range of applications in heat transfer including electronics manufacturing, reactor safety, geothermal energy and most recently, science-based nuclear weapon stewardship. His great strength lies in his ability to conceive and lead multi-disciplinary research and develop programs to investigate complex processes, and then extract physical insights from these to develop practical engineering solutions. A hallmark of his problem solving approach is the synergistic use of analysis, experimentation and numerical simulation.

He held a broad leadership role in advancing experimental strategy to achieve the validation of ASC models for assessment and qualification of nuclear weapons. He served as the key interface between the Sandia model and simulation (M&S) community and the nuclear weapon engineering community to implement strategy to validate M&S tools and to integrate M&S into nuclear weapon qualification, e.g. W76-1. From 2001 to 2004 he served as the Senior Advisor to the Director of the Office of Stockpile Assessments and Certification (Dr. Kevin Greenaugh) at NNSA/DOE, Washington DC.

In 1996 he was elected Fellow of ASME (American Society of Mechanical Engineers) in recognition of his sustained contribution to the Mechanical Engineering profession. He received the Sandia Employee Recognition Award in 1997 (Individual Technical Excellence) and 1999 (Team). He served an Associate Editor of the *Journal of Heat Transfer* from 1999 to 2002. He is a recipient of the 2004 Asian American Engineers of the Year Award given by the Chinese Institute of Engineers, USA.

He started his professional career at AT&T in 1971 and joined Sandia Labs in 1977. A summary of his ***key accomplishments*** are given below:

- ***Fundamentals of Buoyancy-Induced Flow***
  His Ph.D. research in turbulent thermal convection is a classical reference in the field.
- ***Electronics Assembly and Manufacturing* (1971-1976)**
  He co-invented the "Condensation Soldering" process and contributed to the initiation of modeling and simulation of transport processes in electronic materials manufacturing at AT&T. (6 Patents)
- ***Nuclear Reactor Safety (NRC, DOE & OECD) and Geothermal Energy (DOE)* (1977-1996)**
  He developed key facilities and conducted experiments and simulations in coremelt/material interaction, ex-vessel boiling for accident mitigation, and creep rupture of reactor pressure vessels under severe accident conditions. He demonstrated the feasibility of magma energy extraction and contributed to the "High Energy Gas Fracturing" technology for geothermal well stimulation.
- ***Nuclear Weapon Safety and Qualification - Model Validation Strategy* (1996-Present)**
  He participates in Sandia corporate level strategic alignment of ASCI and the needs of weapon engineering, and led a multi-disciplinary team in developing a shared vision between the M&S and weapon engineering communities integrating M&S into the W76-1 Qualification Plan.
  He coordinated, initiated and participated in model validation projects for abnormal thermal environments including fire environment characterization and thermal response modeling.
  Currently, he serves as the Sandia technical Coordinator for the NNSA Weapons Systems Engineering Assessment Technology Campaign (Campaign 6 of the Engineering Campaign).

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Experience

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Intergovernmental Personnel Assignee- Digital Instrumentation and Controls Engineer

- Supported the Digital Instrumentation and Controls Branch in the Office of Regulatory Research by planning, developing, organizing, and coordinating research projects concerning safety aspects of digital systems in commercial nuclear power plants.
- Recent research includes identifying and analyzing failure modes in digital systems and digital system risk quantification issues.

2005-2008 Sandia National Laboratories Albuquerque, NM

Nuclear Engineer, Member of Technical Staff

- Supported Nuclear Risk and Reliability group by conducting reliability and vulnerability assessments of reactor systems.
- Participated in advanced Probabilistic Risk Assessment research including investigation of severe accident uncertainty propagation methods, methodologies to include passive safety features of new reactors, and dynamic methodologies for digital instrumentation and control systems.
- Experienced programming and developing applications on multiple control system platforms. Developed and implemented data acquisition application for Insulation Resistance Measurement System (IRMS) for cable fire experiments and for cyber security control platform penetration testing.

2003-2005 National Instruments Austin, TX

Mechanical Engineering Co-op

- Designed electronics used in industrial and academic data acquisition, signal processing, and control applications.
- Duties include circuit board layout, designing mechanical packaging, and ensuring thermal and mechanical integrity through modeling, prototyping, and environmental/benchmark testing.
- Experience integrating hardware and software applications to produce solutions for automated data acquisition and monitoring of test applications.

Education

2002–2005 The University of Texas at Austin Austin, TX

- B.S. in Mechanical Engineering

2005–2007 Georgia Institute of Technology Atlanta, GA

- M.S. in Nuclear and Radiological Engineering,
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Publications

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UNIVERSITY at BUFFALO, the STATE UNIVERSITY of NEW YORK, Buffalo, New York
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2002 – 2007: *Assistant Professor*

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1998 – 2002: *Senior Member of the Technical Staff (SMTS)*

Purdue University — West Lafayette, Indiana
1993 – 1998: *Research Assistant*
1994 – 1998: *School of Mechanical Engineering Computer Consultant*

HONORS AND AWARDS

National Science Foundation Career Award (2004)
Honorary Member, PI TAU SIGMA, National Mechanical Engineering Honor Society (2004)
Sandia National Laboratories Award for Excellence (2002)
Sandia National Laboratories Award for Excellence (2001)
Air Force Office of Scientific Research fellowship winner for the First Annual International Conference on DNS/LES (1997)
Graduated SUMMA CUM LAUDE from SUNY at Buffalo (1993)
Honor Undergraduate Student Award, SIGMA GAMMA TAU (1993)
President, SIGMA GAMMA TAU, National Aerospace Honor Society (1993)
Member, TAU BETA PI, Engineering Honor Society (1992)
Member, SIGMA GAMMA TAU, Aerospace Honor Society (1992)
Member, National Golden Key Honor Society (1991)
Instrument Society of America Scholarship (1991)

Dean's List every semester at college (1988-1993)
Rochester Industrial Engineering Award (1988)

PROFESSIONAL MEMBERSHIPS AND ACTIVITIES

Technical Chair Member, Solid Propellants and Combustion Committee, American Institute of Aeronautics and Astronautics (2000-2007)
Technical Chair Member, K-11 Fire and Combustion Committee, American Society of Mechanical Engineers (2000-present)
Member, American Society for Engineering Education (2002-present)
Member, American Society of Mechanical Engineers (1994-present)
Member, American Physical Society (1994-present)
Member, The Combustion Institute (1994-present)
Member, National Society of Professional Engineers (1992-present)
Member, SAE International (2007-present)
Member, American Institute of Aeronautics and Astronautics (1990-present)
Reviewer for: Journal of Fluid Mechanics, AIAA Journal, Combustion Science and Technology, International Journal of Multiphase Flows, Atomization and Sprays, International Journal for Numerical Methods in Fluids, Journal of Heat Transfer, International Journal of Heat and Mass Transfer, Journal of Composite Materials, International Journal for Multiscale Computational Engineering, Journal of Fluids Engineering, National Science Foundation, American Chemical Society

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10. **Shihn, H.** and DesJardin, P.E., "Near-Wall Modeling of a Heated Vertical Wall Using One-Dimensional Turbulence", *Int. J. of Heat and Mass Transfer*, **50**, pp. 1314-1327 (2007).

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18. Yoon, S. Hewson, J. C., DesJardin, P. E., Glaze, D. J., Black, A. R. and Skaggs, R. R., "Numerical Modeling and Experimental Measurements of a High Speed Solid-Cone Water Spray for use in Fire Suppression Applications," *Int. J. Multiphase Flows*, **30**, pp. 1369-1388 (2004).

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20. DesJardin, P.E. and Frankel, S.H., "Large Eddy Simulation of Soot Formation in the Near-Field of a Strongly Radiating Nonpremixed Acetylene-Air Turbulent Jet Flame," *Combustion and Flame*, **119**, pp. 121-132 (1999).

21. DesJardin, P.E. and Frankel, S.H., "Large Eddy Simulation of a Nonpremixed Reacting Jet: Application and Assessment of Subgrid-Scale Combustion Models," *Physics of Fluids*, **10,** pp. 2298-2314 (1998).

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23. DesJardin, P.E. and Frankel, S.H., "Assessment of Turbulent Combustion Submodels Using the Linear Eddy Model," *Combustion and Flame*, **104**, pp. 343-357 (1996).

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1. **Luo, C.** and DesJardin, P.E., "Thermo-Mechanical Damage Modeling of Woven Composite Laminates from Fire Environments," New Castle, UK, July 10-11, in <u>Composites in Fire 5</u>, Composites Link Limited, http://compositelink.com/index.php (2008).

2. **Carrara, M. C.** and DesJardin, P.E., "Application of the Two-Phase Filtered Density Function Approach for LES of a 2D Droplet Laden Turbulent Mixing Layer," Third International Conference on Computational Methods in Multiphase Flows, Portland, MA, October 31 – November 2, in <u>Computational Methods in Multiphase Flows III</u>, editors A.A. Mammoli and C.A. Brebbia, WIT Press, Southhampton, Boston (2005).

3. **Carrara, M. C.** and DesJardin, P.E., "Formulation of a Two-Phase Filtered Density Function Approach for Large Eddy Simulation," Third International Conference on Computational Methods in Multiphase Flows, Portland, MA, October 31 – November 2, in <u>Computational Methods in Multiphase Flows III</u>, editors A.A. Mammoli and C.A. Brebbia, WIT Press, Southhampton, Boston (2005).

4. DesJardin, P. E., **Luo, C. and Xie,** W., "Numerical Simulation of Composite Structure Response from a 2D Fire Plume," New Castle, UK, September 15-16, in <u>Composites in Fire</u>

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12. **Carrara, M. D.** and DesJardin, P.E., "Two-Phase Filtered Density Function Approach for Large Eddy Simulation of a Combusting Aluminum Particulate Laden 2D Mixing Layer," 18*th* Engineering Mechanics Division Conference, Virginia Tech., Blacksburg, VA, June 3-6 (2007).

13. **Godoy, W.** and DesJardin, P.E., "Radiative Heat Transfer in Time Evolving Polydisperse Water Spray for Fire Suppression Environments," 5*th* Int. Seminar on Fire & Explosion Hazards, Edinburgh, UK, April 23-27 (2007).

14. **Kumar, A.** and DesJardin, P.E., "A Reaction Progress Variable Approach for LES of Strongly Radiating Flames," 5*th* Int. Seminar on Fire & Explosion Hazards, Edinburgh, UK, April 23-27 (2007).

15. **Godoy, W.** and DesJardin, P.E., “Radiative Properties for Fire Suppression Environments using a Correlated-k Method,” ASME paper IMECE 2005-81710, International Mechanical Engineering Congress and Exposition, Orlando, FL, November 5-11 (2005).

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17. **Luo, C.** and DesJardin, P. E., “Themo-Mechanical Damage Modeling for a Glass-Fiber Phenolic-Resin Composite Material,” ASME paper IMECE 2005-81719, International Mechanical Engineering Congress and Exposition, Orlando, FL, November 5-11 (2005).

18. **Shihn H.** and DesJardin, P. E., “Modeling Heat Transfer from a Vertical Isothermal Plate using One-Dimensional Turbulence Stochastic Mixing Model of Turbulence,” ASME paper IMECE2005-82914, International Mechanical Engineering Congress and Exposition, Orlando, FL, November 5-11 (2005).

19. Yoon, S. and DesJardin, P. E., “Modeling Spray Impingement using Linear Stability Theories for Droplet Shattering,” AIAA paper 2005-3588, 41st Joint AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit (2005), Tucson AZ, July 10-13 (2005).

20. **Luo, C. and Xie, W.** and DesJardin, P.E., “Numerical Simulation of Composite Structure Response from a Fire Plume,” Society for the Advancement of Material and Process Engineering (SAMPE) 2005 Symposium & Exhibition, Long Beach, CA, April 5-7 (2005).

21. **Carrara, M. D.** and DesJardin, P. E., “On Subgrid Scale Modeling of Evaporating Droplets using Probability Density Function Methods,” AIAA paper 2005-1426, 43rd AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 10-13 (2005).

22. **AlSalem, K.,** DesJardin, P. E., Taulbee, D. B. “Hybrid DRP-BEM Method for Acoustics of Buoyancy Driven Plumes,” AIAA paper 2005-0605, 43rd AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 10-13 (2005).

23. **Shihn, H.** and DesJardin, P. E., “Near-wall modeling for Vertical Wall-fires Using One-dimensional Turbulence,” ASME paper IMECE2004-59861, International Mechanical Engineering Congress and Exposition, Anaheim, CA, November 13-19 (2004).

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25. **George, P.** and DesJardin, P.E., “Towards a Mechanistic Model for Aluminum Particle Combustion,” NHTC paper HT2003-47499, ASME National Heat Transfer Conference, Las Vegas, NV, July 20-23 (2003).

26. DesJardin, P.E., Presser, C., Disimile, P.J. and Tucker, J.R., “A Phenomenological Droplet Impact Model for Lagrangian Spray Transport,” AIAA paper 2003-1322, Presented at the 41st AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 6-9 (2003).

27. Domino, S.P, DesJardin, P.E. and Suo-Anttila, J., “Development of a Smoke Transport Model to Enhance the Certification Process for Cargo Bay Smoke Detection Systems,” 7th

International Symposium on Fire Safety Science, Worcester, Massachusetts, June 16-21 (2002).

28. DesJardin, P.E., Nelsen, J., Ghee, T., "On the Development of a Subgrid Scale Clutter Model," AIAA paper 2002-0984, 40th AIAA Aerospace Science Meeting and Exhibit, Reno, NV, January 14-17 (2002).

29. Presser, C., Widmann, J.F., DesJardin, P.E. and Gritzo, L.A., "Measurement and Numerical Prediction of Homogeneous Turbulent Flow over a Cylinder: A Baseline for Droplet-Laden Flow Studies," 40th AIAA Aerospace Sciences Meeting and Exhibit, Reno, NV, January 14-17 (2002).

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35. **Ruggirello, K.** and DesJardin, P.E., "Post Detonation Dispersal and Ignition of Aluminized Explosives," Combustion Institute / Canadian Section, Spring Technical Meeting, Toronto, Canada, May 11-14, (2008).

36. **Xie, W.** and DesJardin, P.E., "New Insights into Upward Flame Spread using 2D Direct Numerical Simulations," Combustion Institute / Canadian Section, Spring Technical Meeting, Toronto, Canada, May 11-14, (2008).

37. **Xie, W**. and DesJardin, P.E., "Numerical Simulation of Concurrent Flame Spread Over PMMA Slab with Different Thicknesses and Orientations," 9th U.S. National Congress on Computational Mechanics (USNCCM IX), San Francisco, CA**,** July 23-26 (2007).

38. **Luo, C.** and DesJardin, P.E., "Thermo-mechanical Damage Modeling for Composite Materials," 9th U.S. National Congress on Computational Mechanics (USNCCM IX), San Francisco, CA**,** July 23-26 (2007).

39. DesJardin, P. E., “Fire Protection Opportunities for Next Generation Buildings using Sensor Technology,” Joint US-Japan Workshop on Next Generation Buildings, Honolulu, HI, Feb. 26-27, (2007).

40. **Kumar, A**. and DesJardin, P. E., “A Reaction Progress Variable Approach for LES of Sooty Flames,” APS Fluid Dynamics Meeting, Tampa, FL, November 19-20, (2006).

41. **Shihn, H.** and DesJardin, P. E., “Near-wall SGS modeling for LES of an Isothermal Wall using ODT,” APS Fluid Dynamics Meeting, Tampa, FL, November 19-20, (2006).

42. **Carrara, M. D.** and DesJardin, P.E., “Two-Phase Filtered Density Function Approach for Large Eddy Simulation of a Water Droplet Laden 2D Mixing Layer,” APS Fluid Dynamics Meeting, Chicago, IL, November 20-22 (2005).

43. **Shihn, H.** and DesJardin, P.E., “One-Dimensional Turbulence Modeling for a Heated Vertical Wall”, APS Fluid Dynamics Meeting, Chicago, IL, November 20-22, (2005).

44. **Carrara, M. D.** and DesJardin, P. E., “A Probabilistic Approach to Modeling Separated Two-Phase Flows for Large Eddy Simulation,” APS Fluid Dynamics Meeting, Seattle, WA, November 21-23 (2004).

45. **Shihn, H.** and DesJardin, P.E., “Simulation of a Vertical Wall Fires with One-Dimensional Turbulence Modeling”, Combustion Institute / Canadian Section, Spring Technical Meeting, Kingston, Ontario, Canada, May 9-12, (2004).

46. **Luo, C.** and DesJardin, P.E., “Towards a Thermo-Mechanical Damage Model for Composite Structures,” Combustion Institute / Canadian Section, Spring Technical Meeting, Kingston, Ontario, Canada, May 9-12, (2004).

47. Yoon, S.S., Hewson, J.C., DesJardin, P.E., Glaze, D. J., Black, A. R., Skaggs, R. R., “On the modeling of a solid-cone water spray,” ILASS Americas, 17^{th} Annual Conference on Liquid Atomization and Spray Systems, Arlington, VA, May (2004).

48. **Aranha, R.S.** and DesJardin, P.E., “Flow Instability Dynamics of Helium Plumes,” IMECE paper International Mechanical Engineering Congress and Exposition, Washington, D.C., November 11-16 (2003)

49. DesJardin, P.E., “On the Modeling of the Flamelet Model Conditional Dissipation Rate for use in LES of Pool Fires,” 3^{rd} Joint Meeting of the U.S. Sections of the Combustion Institute, Chicago, IL, March 16-19 (2003).

50. Smith, T., Shadid, J., DesJardin, P.E. and Lin, P., “Large-Eddy Simulation of a Pool Fire Using a Galerkin Least-Squares Finite-Element Method,” Computational Methods for Multidimensional Flows Conference, Heidelberg, Germany, December 2-4 (2002) .

51. Bell, R. and DesJardin, P.E., “CTH Time Step Modification Based on Pressure Gradient Scaling,” Presented at the Fourth Biennial Tri-Laboratory Engineering Conference on Computational Modeling, Albuquerque, NM, October 22-24 (2001).

52. DesJardin, P.E., Tiesen, S.R., Shienson, R., Maranghides, A. and Ayers, S., "Pool Fire Numerical Simulation and Modeling of Water Spray Suppression," Water Mist Fire Suppression Workshop, Colorado School of Mines, Golden, CO, October 10-11 (2001).

53. DesJardin, P.E., Roy, C.J. and Smith, T.M. "Large Eddy Simulation of a Turbulent Reacting Plume," Presented at the International Conference on Numerical Combustion, Amalia Island, FL, March 5-8 (2000).

54. DesJardin, P.E., "Large Eddy Simulation of a Buoyant Turbulent Plume," Presented at the APS Fluid Dynamics Meeting, New Orleans, LA, November 19-24 (1999) .

55. DesJardin, P.E. and Frankel, S.H., "Large Eddy Simulation of Soot Formation in a Strongly Radiating Nonpremixed Acetylene-Air Jet Flame using Parallel Computations," Central States Section of the Combustion Institute, KN, June (1998).

56. DesJardin, P.E. and Frankel, S.H., "A New Subgrid-Scale Combustion Model for Large Eddy Simulation," APS Fluid Dynamics Meeting, San Francisco, CA, November 23-25 (1997) .

57. DesJardin, P.E. and Frankel, S.H., "Large Eddy Simulation of a Nonpremixed Reacting Jet: Effects of Soot and Radiation," First AFOSR International Conference on DNS/LES (FAICDL), Ruston, LA, August 4-8 (1997) .

58. DesJardin, P.E. and Frankel, S.H., "Towards Large Eddy Simulation of a Sooty Coflow Planar Jet Diffusion Flame," Central States Section of the Combustion Institute, Point Clear, AL, April 27-29 (1997).

59. DesJardin, P.E. and Frankel, S.H., "Large Eddy Simulation of a Sooty Spatially Developing Planar Jet," APS Fluid Dynamics Meeting, Syracuse, NY, November 24-26 (1996).

60. DesJardin, P.E. and Frankel, S.H., "Numerical Simulations and Modeling of Homogeneous and Nonhomogeneous Turbulent Reacting Flows: SLFM and CMC Validity," Joint Central, Western, and Mexican Sections of the Combustion Institute, San Antonio, TX, April 23-26 (1995) .

61. DesJardin, P.E. and Frankel, S.H., "Linear Eddy Modeling of Nonequilibrium Chemistry in Homogeneous Turbulence with Nonpremixed Reactants," APS Fluid Dynamics Meeting, Irvine, CA, November 18-21 (1995).

62. DesJardin, P.E. and Frankel, S.H., "Numerical Investigation of Turbulent Combustion Submodels," APS Fluid Dynamics Meeting, Atlanta, GE, November 20-22 (1994).

63. DesJardin, P.E. and Frankel, S.H., "Numerical Validations of Turbulent Combustion Submodels," Central Section Meeting of the Combustion Institute, Madison, WI, June 5-7 (1994).

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64. DesJardin, P.E., Baer, M.R., Bell, R. L. and Hertel, E. S. "Towards Numerical Simulation of Shock Induced Combustion using Probability Density Function Approaches," Sandia National Laboratories Technical Report, SAND2002-2175 (2002).

65. DesJardin, P.E. and Gritzo, L.A., “A Dilute Spray Model for Fire Simulations: Formulation, Usage and Benchmark Problems,” Sandia National Laboratories Technical Report, SAND2002-3419 (2002).

66. Schmidt, R. C., Smith, T.M., DesJardin, P.E., Voth, T.E., Christon, M.A., Kerstein, A.R. and Wunsch, S.E., ”On the Development of the Large Eddy Simulation Approach for Modeling Turbulent Flow: LDRD Final Report,” Sandia National Laboratories Technical Report , SAND2002-0807 (2002).

67. Gritzo, L.A., Strickland, J.H. and DesJardin, P.E., “Radiation in a Emitting and Absorbing Medium: A Gridless Approach,” Sandia National Laboratories Technical Report, SAND2000-0960 (2000).

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EDUCATION

University of Utah
Ph.D., Chemical Engineering (Professor P. J. Smith)
December 1999
•"Methods Toward Improved Simulations for the Oxides of Nitrogen in Pulverized-Coal Furnaces"

University of Washington
Autumn 1994 - Spring 1995

University of Utah
B.S. Chemical Engineering, June 1994

PRINCIPLE MEMBER OF THE TECHNICAL STAFF
SANDIA NATIONAL LABORATORIES (October, 2005 - Present)

- On going responsibilities as Principle Investigator for SIERRA/Fuego/Syrinx (a low Mach number, heterogenous toplogy, control-volume-finite-element, massively parallel turbulent reacting flow code) that includes both technical leadership and project management.

SENIOR MEMBER OF THE TECHNICAL STAFF
SANDIA NATIONAL LABORATORIES (July, 2001 - September 2005)

- Advanced numerical and physical model development for CFD fire simulation codes.
- Promotion to Principle Investigator of SIERRA/Fuego/Syrinx starting in 2003.

POSTDOCTORATE APPOINTEE
SANDIA NATIONAL LABORATORIES (May, 2000 - July, 2001)

- Development of a transient turbulent Finite Volume CFD code capable of modeling smoke transport in cargo bay compartments.
- Half time code developer on SIERR/Fuego, within the object oriented architecture, SIERRA.
- Advanced numerical and physical model development for CFD fire simulation codes.

RESEARCH ASSOCIATE
UNIVERSITY OF UTAH with Professor Philip J. Smith (1995-1999)

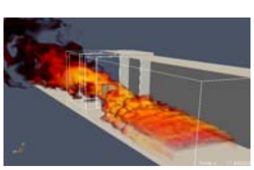
- Implemented an advanced carbon burnout model within a multiphase turbulent reacting flow code.
- Researched the intimate coupling between carbon burnout and NO_x emissions in pulverized coal furnaces.
- Implementation of improved nitrogen release rates for increased accuracy of gas phase nitrogen mass source terms by the incorporation of additional turbulent progress variables; implementation and research of a joint β-PDF mixing model.

PRIVATE CONSULTING EXPERIENCE

- Expert CFD witness for the Commerce and Industry Insurance Company.
- Contracted by EM Assist to develop a computer program capable of calculating multicomponent evaporation rates.

INDUSTRIAL EXPERIENCE

- Summer professional intern at Gore Hybrid Technologies, of W.L Gore.



170,000,000 combined degree-of-freedom SIERRA/Fuego/Syrinx/Calore simulation; shown is the volume rendered temperaturefield.

- Research towards the increased biocompatibility of mammalian cells at a PDMS surface.

TEACHING EXPERIENCE

- Two time teaching assistant for University of Utah graduate multicomponent mass transfer class. Topics taught: Estimation of multicomponent diffusion coefficients; Numerical solution techniques for exact Generalized Maxwell-Stefan equations; General review of boundary layer theory and the effects of simultaneous heat and mass transfer; Guest lecturer for U of U undergraduate fundamentals of combustion class, CHFEN 5153."Fundamentals of Turbulent Reacting Flow Simulation".

COMPUTER SKILLS and CFD CODES

- Proficient in many computer operating systems and software platforms including Unix, Windows and Windows N.T.; languages of FORTRAN, C, and C++.
- CFD codes SIERRA/Fuego FLUENT, FLUENT/UNS, Banff, Glacier; mesh packages of GeoMesh and Tgrid.

AWARDS and HONORS

- Western States Section of The Combustion Institute Student Award. Presented to outstanding graduate students for technical conference presentations of accepted research papers.
- Research Assistantship award from the University of Washington and the University of Utah.
- Multiple Dean's List awards as an undergraduate chemical engineering student.
- Undergraduate Division I full athletic scholarship (soccer).

PAPERS and PRESENTATIONS

•C. Moen, S. P. Domino and G. Wagner, "Approximate Projection Methods and Time Integration Stability". Third MIT Computational Fluid and Solid Mechanics, paper number 176-313, 2005.

•C. Moen and S.P. Domino, "A Review of Splitting Errors for Approximate Projection Methods", CFD2003, Orlando, FL, 2003.

•C. Moen G. H. Evans, S.P. Domino and S. Burns, "A Multi-Mechanics Approach to Computaitonal Heat Transfer", International Mechanical Engineering Congress and Exposition, New Orlean, Gaithersburg, MD, 2001.

•S. P. Domino and P. J. Smith, "State Space Sensitivity to a Prescribed PDF Shape in Coal Combustion Systems: Joint β-PDF vs. Clipped Gaussian PDF", *Proc. Combust. Institute*: 20, **2001** in press.

•D. Blake, S.P. Domino, W. Gill, L. Gritzo, J. Williams, "Initial Development of Improved Aircraft Cargo Compartment Fire Detection Certification Criteria", Proc. of the 12th Conference on Automatic Fire Detection, Gaithersburg, MD, 2001.

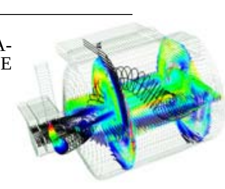
•S. P. Domino and P. J. Smith, "Burnout Model Validation in Coal Combustion Simulations", *ASME, HTD*, (Publication) HTD; **1999**; v.364-2, p.395.

•S. P. Domino and P. J. Smith, "Loss on Ignition in Coal Combustion Simulations", submitted to *Combustion and Flame*. Second draft corrections are in process.

•S. P. Domino and J. M. Veranth, "Modeling of Elemental Vaporization and Partitioning During Pulverized-Coal Combustion", paper and technical presentation, The 17th Annual Conference of the American Association for Aerosol Research, Cincinnati, Ohio, June 22-26, 1998.

•S. P. Domino and P. J. Smith, "Improved NO_x predictions in Pulverized Coal Furnaces", Paper and technical presentation, The Fall Meeting of the Western States Section, The Combustion Institute, Pittsburgh, South Coast Air Quality Management District, Diamond Bar, Ca., October 23-24, 1997.

•S. P. Domino and P. J. Smith, "Thermal Annealing, Reactivity Distribution and Ash Inhibition Effects on Char Burnout: A Comparison of 3-D Turbulent Multiphase CFD Theoretical Burnout Calculations and Experimental Burnout Measurements", Poster Session, American Flame Research Committee Meeting, Salt Lake City, UT, April 1-3, 1998.



SIMULATED NO CONCENTRATION PROFILES IN A CYCLONE REACTOR

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Experience

Sandia National Laboratories - Albuquerque, New Mexico

Current Position: Principal Member of Technical Staff

Research Assignments

10/96 to present

- Experimental investigations (TGA, FTIR, GC-MS, DSC) to determine mechanisms and kinetics controlling thermal decomposition of polymer materials pertinent to critical weapon components and fire modeling. Principal investigator for four Sandia projects including Campaign 6 Foam Decomposition Chemistry Project, which involves activities in several Sandia organizations, as well as work at BYU and GA Tech. Project also involves collaborative work with the All Russian Research Institute of Automatics (Moscow) and the Mendeleev Institute (Moscow).
- Development of multi-component, 3-D models/codes predicting base metal dissolution and inter-metallic compound growth in solder joints (models/codes for manufacturing and reliability applications). Coordinator/spokesperson for Sandia's ASCI Solder Program, which involves activities in several Sandia organizations.

10/88 to 09/96

- Experimental and theoretical work to determine chemical and physical processes controlling solder joint aging and to develop 1-D computer codes for design and reliability analyses. Coordinated experiments with model and code development.
- Development of advanced diagnostics for studying high-temperature, rapid thermal decomposition of high explosives using TOFMS and thin-film samples. Developed vapor deposition equipment and techniques for preparing samples.
- Experimental investigations to determine condensed-phase decomposition chemistry of high explosives using FTIR and thin-film samples.

12/76 to 09/88

- Experimental investigation of reaction kinetics and development of ignition models for pyrotechnic materials involving both gas-solid and liquid-solid reactions.
- Development of advanced tracer techniques for studying pore structures in granular materials and providing more detailed pore structure characterization.
- Experimental investigations of radio-nuclide sorption and transport in geologic media.

United States Army

Assignments

09/71 to 08/73: Staff officer, U. S. Army Combat Developments Command, Field Artillery Agency, Ft Sill. OK. Honorably discharged.

09/70 to 09/71: Assistant Operations Officer 1st Bn 82nd Field Artillery, U. S. Army Vietnam. Promoted to captain.

02/70 to 09/70: Field Artillery Basic (Ft Sill, OK), Ranger School (Ft Benning, GA)

08/68 to 02/70: Commissioned 2Lt. Granted leave for graduate school. Promoted to 1Lt

Education

Ph. D.	Chemical Engineering	1977	University of Texas at Austin
M. S.	Chemical Engineering	1973	University of Arizona
B. S.	Chemical Engineering	1968	University of Arizona

Professional Societies

American Institute of Chemical Engineers - member 1968 to present

American Chemical Society - member 1976 to present

The Minerals, Metals and Materials Society - member 1997 to present

Interests

Martial arts, skiing, canoeing, history/military history

Publications

List enclosed

References

Will be furnished on request

PUBLICATIONS

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P. T. Vianco, K. L. Erickson, P. L. Hopkins, and A. C. Kilgo , “Computational Model for Predicting Solid-State Reactions in Porous Materials: Case Study – the Reliability of Hybrid Microelectronics,” National Space & Missle Materials Symposium 2002, Colorado Springs, CO, 24-27 June 2002.

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Educational Background

University of California, Berkeley	Mechanical Engineering	B.S.	1990
University of California, San Diego	Engineering Sciences	M.S.	1993
University of California, San Diego	Engineering Sciences	Ph.D.	1997

Thesis: *Pollutant Emissions from Nonpremixed Hydrocarbon Flames*
Advisor: Prof. Forman A. Williams

Professional Experience:

9/02 – present: *Principal Member of the Technical Staff*, (11/07-present), *Senior Member of the Technical Staff*, (9/02-11/07), Sandia National Laboratories, Albuquerque, NM.

12/98 – 9/02: *Postdoctoral Appointee, Limited-Term Member of Technical Staff*, Sandia National Laboratories, Livermore, CA.

8/97 – 12/98: *Visiting Postdoctoral Chemist,* Lawrence Berkeley National Laboratory, Berkeley, CA.

9/91 – 8/97: *Research Associate,* University of California, San Diego, CA.

1/95 – 3/95: *Teaching Assistant,* University of California, San Diego, CA.

9/94 – 11-94: *Visiting Researcher*, Institut fur Technische Mechanik, RWTH-Aachen, Germany.

8/93-12/93: *Visiting Researcher*, Department of Thermal Energy and Hydropower, The Norwegian Institute of Technology, Trondheim, Norway.

8/90 – 8/91: *Mechanical Engineer,* Systron-Donner Safety Systems Division, Concord, CA.

Current and Recent Research Projects:

Fundamental studies of turbulent nonpremixed flame evolution with emphases on trace species/pollutant formation and destruction and on localized extinction and reignition.

Developing models for the transport of aerosols relative to gases, focusing on the varying thermochemical state.

Implementing conditional moment closure models into production multiphysics analysis code to track enthalpy and aerosol evolution in complex geometries where substantial conjugate heat transfer occurrs.

Developing models for multi-source mixing evolution when length and time scales vary between sources.

Modeling spray evolution using Lagrangian particle tracking methods. Developing improved models for particle combustion and for droplet impact.

Developing models of the thermochemistry of metal oxidation and metal-metal alloying reactions to predict the thermochemical evolution of metals in high-temperature environments.

Analyzing the sensitivity of ignition to the mixing process and fuel composition with model for full range of length and time scales. Using this to develop control strategies for HCCI engines.

Modeling the dynamics of localized extinction and reignition in turbulent flames with stochastic modeling.

Development of detailed chemical-kinetic mechanisms and simplified models related to main-flame chemistry and pollutant emissions from flames.

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S. S. Yoon, J. C. Hewson, P. E. DesJardin, D. J. Glaze, A. R. Black, R. R. Skaggs, “Numerical modeling and experimental measurements of a high speed solid-cone water spray for use in fire suppression applications,” *International Journal of Multiphase Flow*, 30(11):1369-1388, 2004.

J. C. Hewson and A. R. Kerstein, “Local Extinction and Reignition in Nonpremixed Turbulent $CO/H_2/N_2$ Jet Flames,” *Combust. Sci. Tech*., 174 (5-6):35-66, 2002.

J. C. Hewson and A. R. Kerstein, “Stochastic Simulation of Transport and Chemical Kinetics in Turbulent $CO/H_2/N_2$ Flames,” *Comb. Theory Modeling*, 5:669-697, 2001.

J. C. Hewson and F. A. Williams, “Rate-Ratio Asymptotic Analysis of Methane-Air Diffusion Flame Structure for Predicting Production of Oxides of Nitrogen,” *Combust. Flame*, 117: 441-476, 1999.

Other Recent Activities

Member of the Organizing Committee for the Workshop on Fire Models and Validation (2007, 2006) and Workshop on Heat Transfer in Fires (2007, 2006, 2005, 2004, 2003) These annual workshops are organized to provide a venue for the international research community to address physics modeling and validation in fire environments.

Member of the Organizing Committee for the International Workshop on Combustion-Generated Fine Carbon Particles (Anacapri, Italy), May 13-16, 2007. This workshop was organized to bring together the international soot research community to assess and review recent progress.

Moderator for Department of Energy Science Bowl, an annual outreach program to high school and middle school students encouraging excellence in the sciences (1999-2007)

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Vernon F. Nicolette, PhD

Work Experience

Sandia National Laboratories (1985 – present)
Job Title: Principal Member of Technical Staff

- Principal investigator (PI) with project management responsibilities
  - Product manager for the Fuego fire code (2007 – 2008)
  - PI for Fuego propellant fire code V&V (2007 – 2008)
- CFD computer code development
  - Developed the Vulcan CFD fire code (1993 – 2008)
  - Developed the Gray Gas model for predicting radiation boundary layers in convective environments (1989 – 1990)
  - Developed a thermal battery computer code (1990 – 1993)
  - Developed a computer code for simulation of hydrogen burns in nuclear reactor accident environments (1985 – 1989)
- Numerical and analytical studies of fires, buoyant flows, and heat transfer
  - Numerous studies of accident environments and thermal response

Accomplishments
Designated "Founding Father" of the Fire Science & Technology Program at Sandia National Laboratories

Activities
Member of ASME, IAFSS. Co-chairman of Weapons Effects Strategic Collaboration Fire Working Group.

Interests
Fires and combustion environments (nuclear facilities, accidents, aircraft), thermal radiation, probabilistic risk assessment, verification and validation

Hobbies
Running, tennis, bible study. Youth pastor (1997 – 2007).

Education

University of Notre Dame
Department of Aerospace and Mechanical Engineering
Notre Dame, Indiana
Dates: 1984 – 1985
Degree: Postdoctoral research on buoyant flows and natural convection

University of Notre Dame (received scholarship)
Department of Aerospace and Mechanical Engineering
Notre Dame, Indiana
Dates: 1980– 1984
Degree: Doctor of Philosophy in Mechanical Engineering. Dissertation: Transient Natural Convection in Enclosures (Advisor: K.T. Yang)

University of California at Berkeley (received scholarship)
Department of Nuclear Engineering
Berkeley, California
Dates: 1979 – 1980
Degree: Master of Science in Nuclear Engineering
Thesis: Two-Phase Fanno Flow Using a Homogeneous Equilibrium Model (Advisor: V.E. Shrock)

University of Notre Dame (received scholarship)
Department of Aerospace and Mechanical Engineering
Notre Dame, Indiana
Dates: 1975– 1979
Degree: Bachelor of Science in Mechanical Engineering

Special Appointments
Visiting Researcher, Norwegian Technical University, Trondheim, Norway (1993 and 1995)
Visiting Scientist, FAA Technical Center, New Jersey (1993 – 1995)

Partial List of Publications

- V.F. Nicolette, S.R. Tieszen, L.A. Gritzo, "Numerical Simulation of Fire in an Aircraft Engine Nacelle," Annual Conference on Fire Research, NIST, Gaithersburg, MD, October 1996.
- V.F. Nicolette, S.R.. Tieszen, and J.L. Moya, "Interfacing Materials Models with Fire Field Models," Proceedings of the 41st SAMPE Symposium, Anaheim, CA, March 1996.
- V.F. Nicolette, "Fire Model Simulations for the Dual Capable Aircraft Program," Sandia National Laboratories report, SAND 2000-1729, Specified Dissemination, Official Use Only, August 2000.
- V.F. Nicolette, "Computational Fire Modeling For Aircraft Fire Research," Sandia National Laboratories report, SAND96-2714, November 1996.
- V. F. Nicolette, W. Gill, and T. K. Blanchet, "Reconciliation of Experimental Observations with Zone Models and Field Models in Large-Scale Non-Conventional Compartment Fires," HT 99-WA/HT-10007, 1999 ASME Int. Mech. Eng. Congress and Exposition (IMECE), Nashville, TN, Nov. 15-20, 1999.
- V.F. Nicolette, S.R. Tieszen, A.R. Black, S.P. Domino, T.J. O'Hern, A Turbulence Model for Buoyant Flows Based on Vorticity Generation, Sandia National Laboratories report, SAND 2005-6273, 2005.
- V.F. Nicolette, Vulcan Simulations of ICFMP Benchmark Exercise 4, Test 3, Sandia National Laboratories report, SAND2006-1721, 2006.
- V.F. Nicolette, K.L. Erickson, and B.E. Vembe, Numerical Simulation of Decomposition and Combustion of Organic Materials, Proceedings of the INTERFLAM Conference, Edinburgh, Scotland, July 5-7, 2004.
- V.F. Nicolette and B.E. Vembe, Numerical Simulation of Solid Material Decomposition and Combustion, SAMPE Conference, Long Beach, CA, May 19, 2004.
- V.F Nicolette, Gritzo, L.A., Moya, J.L., and Tieszen, S.R., "Comparison of Large JP4- and JP8-Fueled Pool Fires," Proceedings of the International Conference on Fire Research and Engineering, Orlando, Florida, September 10-15, 1995, SFPE, Quincy, MA, 1995.
- V.F. Nicolette, A.L. Brown, and A. R. Black (eds.), VULCAN Users Manual, Sandia National Laboratories report SAND2008-1205, 2008.
- V.F. Nicolette and J.C. Hewson, Modeling the thermal environment from ambient atmosphere solid propellant fires, JANNAF Proceedings, Boston, March 2008.
- J.C. Hewson and V.F. Nicolette, Predicting aluminum droplet burning rates with varying oxidizers, JANNAF Proceedings, Boston, March 2008.
- W. Gill, W.W. Erikson, V.F. Nicolette, and J.C. Hewson, Heat flux from ambient air solid propellant fire plumes, JANNAF Proceedings, Boston, March 2008.
- H. Noravian, V.F. Nicolette, K.A. Woodbury, L.E. Reinhart, and N.R. Keltner, Vulcan/SINDA loosely coupled analysis methodology for the NASA/JPL rod calorimeter, JANNAF Proceedings, Boston, March 2008.
- W.W. Erikson, V.F. Nicolette, and W. Gill, Uncertainty in propellant fire heat flux – an experimental and modeling approach, Department of Defense Explosives Safety Seminar, Palm Springs, CA, Aug. 12-14, 2008.
- Brundage, A.L., Kearney, S.P, Donaldson, A. B., Nicolette, V. F., Gill, W, "A Joint Computational and Experimental Study to Evaluate Inconel-Sheathed Thermocouple Performance in Flames", SAND2005-3978, June 2005.
- L. A. Gritzo and V.F. Nicolette, Coupling of Large Fire Phenomenon with Object Geometry and Object Thermal Response, Journal of Fire Sciences, vol. 15, December 1997.
- S.R. Tieszen, V.F. Nicolette, L.A. Gritzo, J.K. Holen, D. Murray, and J.L. Moya, Vortical Structures in Pool Fires: Observation, Speculation, and Simulation, Sandia National Laboratories report, SAND96-2607, 1996.
- Gritzo, L.A., and Nicolette, V.F. "Coupled Thermal Response of Objects and Participating Media in Fires and Large Combustion Systems," Numerical Heat Transfer, Part A, 28:531-545, 1995.
- Gritzo, L.A., Nicolette, V.F., Tieszen, S.R., and Moya, J.L. "Heat Transfer to the Fuel Surface in Large Pool Fires," Transport Phenomenon in Combustion, S.H. Chan, ed., Taylor and Francis, 1995.
- Gritzo, L.A., Gill, W., and Nicolette, V.F., "Estimates of the Extent and Character of the Oxygen-Starved Interior in Large Pool Fires," Very Large Scale Fires, ASTM STP 1336, N.R. Keltner, N.J. Alvares and S.J. Grayson, Eds., American Society for Testing and Materials, 1998.
- Gritzo, L.A., Nicolette, V.F, Moya, J.L., Skocypec, R.D., and Murray, D., "Wind-Induced Interaction of a Large Cylindrical Calorimeter and an Engulfing JP-8 Pool Fire," Proceedings of the Symposium on Thermal Sciences in Honor of Chancellor Chang-Lin Tien, Berkeley, CA, November 14, 1995. Printed by the Department of Mechanical and Industrial Engineering, University of Illinois at Urbana-Champaign.
- Gritzo, L.A., Moya, J.L., Nicolette, V.F, and Gilliland, J., "Characterization of Large JP4 Pool Fires and Heat Fluxes Incident on an Adjacent Flat Surface," Proceedings of the International Conference on Fire Research and Engineering, Orlando, Florida, September 10-15, 1995, SFPE, Quincy, MA, 1995.
- A.L. Brown, K.J. Dowding, V F. Nicolette, and T.K. Blanchat, Fire model validation for gas temperatures and radiative/convective partitioned heat flux, Proc. Int. Assoc. of Fire Safety Science, Karlsruhe, Germany, August 2008.

Tara J. Olivier

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Education:

M.S. in Fire Protection Engineering, Worcester Polytechnic Institute, (WPI) (2007)
B.S. in Mechanical Engineering, WPI (2005)

Relevant Courses: Enhancements to FDS, Combustion, Process Safety Management, Fire Modeling, Failure Analysis, Performance Based Design, Fire Dynamics, Fire Protection Systems, Building Fire Safety, Operations Risk Management

Work Experience:

2005-Present **Member of the Technical Staff, Sandia National Laboratory, Risk and Reliability Analysis Department** Albuquerque, NM

2004-2005 **Volunteer Lab Assistant: Fire Testing for the U.S. Navy** Holden Labs, Holden MA

- Testing the Performance of Fire Fighting Clothing
- Monitoring the Flow Controller and Thermocouples

Research and Professional Experience:

2008 Sodium Fast Reactor Safety Training, Japan Atomic Energy Association
2007 EPRI/NRC-RES Fire PRA Course

Selected Publications:

Olivier, T.J., R.F. Radel, S.P. Nowlen, T.K. Blanchat, and J.C. Hewson, *Metal Fire Implications for Advanced Reactors, Part 1: Literature Review*, SAND2007-6332. Sandia National Laboratories, Albuquerque, NM, October 2007.

Olivier, T.J., T.K. Blanchat, J.C. Hewson, S.P. Nowlen, R.F. Radel, *Metal Fires and Their Implication for Advanced Reactors*, ANS PSA 2008 Topical Meeting- Challenges to PSA during the nuclear renaissance. Knoxville, TN, September 7-11, 2008, on CD-ROM, American Nuclear Society, LaCrange Park, IL (2008).

Professional Activities:

- Member of ANS Trinity Section (2008)
- Member of SFPE (2005-Present)

RESUME

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EDUCATION

PhD — Chemistry, Chemical Engineering and Economics
California Institute of Technology, 1975
Thesis: "Magnetic Behavior of Basic Iron Compounds"

BS — Chemistry
California Institute of Technology, 1970

Engineer-in-Training Certificate, State of California

PROFESSIONAL SOCIETIES

American Chemical Society
American Nuclear Society

- elected to Executive Committee of the Nuclear Installation Safety Division 2004
- Chairman Program Committee for the Nuclear Installations Safety Division 2006-2007
- Vice Chairman Program Committee for the Nuclear installations Safety Division 2006
- secretary Program Committee for the Nuclear Installation Safety Division 2004-2005
- member Program Committee for the Nuclear Installation Safety Division 2001- present

Tau Beta Pi

EXPERIENCE

November 2007 — Theos J. “Tommy” Thompson award from the American Nuclear Society “in recognition of outstanding contributions to the field of nuclear reactor safety”.

June 2002	Elected Fellow of the American Nuclear Society Member of the Program Committee for the Nuclear Installations Safety Division of the American Nuclear Society
June 2001	Distinguished Service Award from US Nuclear Regulatory Commission
1994 - Present	Member, Advisory Committee on Reactor Safeguards U.S. Nuclear Regulatory Commission
1999, 2000	Chairman Advisory Committee on Reactor Safeguards U.S. Nuclear Regulatory Commission
1997, 1998	Vice-Chairman Advisory Committee on Reactor Safeguards U.S. Nuclear Regulatory Commission

As a member of the Advisory Committee, chaired subcommittees on Reactor Fuels, Fire, Human Factors and Reactor Safety Research; served on subcommittees dealing with reactor thermal hydraulics and probabilistic risk assessment.

1998 - Present	Senior Scientist, Nuclear and Risk Technologies Center Sandia National Laboratories

Responsible for organization of Senior Scientists' review of technical issues for Sandia management; consults with the Nuclear Regulatory Commission on international reactor safety research programs (ARTIST, PHEBUS, MASCA); conducts thermal analysis for launch safety analysis for the New Horizons mission to Pluto; part of the international team developing a state-of-the-art report on nuclear aerosols for Organization for Economic Cooperation and Development (OECD).

1992 - 1998	Manager (ML-1) Nuclear Facilities Safety Department Sandia National Laboratories

Responsible for the development of safety research programs for Department of Energy nuclear facilities; development of knowledge-based expert system for facility safety surveys.

Participated in the team conducting The System Requirements Review for the Hanford Tank Waste Remediation System.

Consultant for Chemical Reactions Subcommittee of the Tank Advisory Panel (DOE/EM-36) examining safety issues of radioactive wastes stored by the

Department of Energy.

Served on Experts Group on Risk Acceptance Criteria for In-Facility Personnel, Co-located Workers, and the Public for DOE/EH-10.

Lecturer in the IAEA Severe Accident Analysis and Accident Management Program to Beijing, China.

1991 August-1992 March
Acting Manager Department 6420
Sandia National Laboratories

Managed the work of four divisions involving 58 Sandia employees and about 30 contractors conducting in-pile experiments, out-of-pile experiments and phenomenological modeling of nuclear reactor accidents and the development of plasma-facing components for fusion reactors.

Lecturer for the IAEA Accident Management and Accident Analysis course December 2-13, 1991, South Korea.

1981 – 1991 August Supervisor
Sandia National Laboratories

Supervised the work of about 10 staff members, eight technicians and up to 10 contractors conducting experimental and analytic investigations of severe reactor accident phenomena on behalf of the U.S. Nuclear Regulatory Commission and the Department of Energy; large-scale field tests of core debris/concrete interactions, sodium/concrete interactions, molten aluminum/concrete interactions, melt/water interactions, direct containment heating, and fission product/aerosol interactions with reactor structures were conducted in the division; computer models of sodium/concrete interactions (SLAM), core debris/concrete interactions (CORCON/VANESA), fission product release and transport (VICTORIA), melt flow (PLUGM), concrete dehydration (USINT), and direct containment heating (TCE) were developed for the analysis of severe reactor accidents; methods for quantitative scaling and uncertainty analyses were devised.

1988 March - 1991 November
Member
Department of Energy Advisory Committee on Nuclear Facility Safety (J. Ahearne, Chairman)

Provided the Secretary of Energy advice on the safety of reactor and nuclear facilities operated by or for the DOE; chaired subcommittees dealing with restart of the Savannah River K reactor, Rocky Flats operational safety, and safety issues at the Hanford tank farms.

1988	Member, National Research Council Steering Committee for the Workshop on Chemical Processes and Products in Severe Reactor Accidents (J. Margrave, Chairman)
1986 - 1988	Member, National Research Council Committee to Assess Safety and Technical Issue at Department of Energy Reactors (R. Meserve, Chairman)
1986	Consultant, International Nuclear Safety Advisory Group (IAEA) on the Chernobyl accident.
	Lecturer in IAEA courses on Severe Accident Phenomena held in Rio de Janero, Brazil; Ljubljana, Yugoslavia; Johannesburg and Capetown, South Africa; and Veracruz, Mexico.
1974 - 1981	Staff Member, Chemistry and Metallurgy Division Sandia National Laboratories

Developed techniques for the hot pressing of metallothermic reaction mixtures. Studied the nature of metallothermic reaction ignition.

Conducted experimental studies of high temperature core debris interactions with concrete, steel, firebrick, borax, high alumina cement and magnesia; developed models of the kinetics of concrete decomposition; studied the heat transfer from high temperature melts to steel structures and urania-coated steel structures; developed methods to use x-rays for observing in real time melt interactions with materials.

Served as a consultant to the President's Commission on the accident at Three Mile Island.

Served on a working group for the Rogovin Commission's investigation of the reactor accident at Three Mile Island.

Served as a consultant to the Advisory Committee Reactor Safeguards Subcommittee on Class 9 accidents (D. Okrent, Chairman) and control room habitability (D. Moeller, Chairman).

PUBLICATIONS

1. D. A. Powers and H. B. Gray, "Characterization of the Thermal Dehydration of Zirconium Oxide Halide Octahydrates", **Inorganic Chemistry *12***,(1973) 2721.

2. D. A. Powers, G. R. Rossman, H. J. Schugar, and H. B. Gray, "Magnetic Behavior and Infrared Spectra of Jarosite, Basic Iron Sulfate, and their Chromate Analogs", **Journal of Solid State Chemistry *13***, (1975) 1.

3. J. A. Thick, C. C. Ou, D. A. Powers, B. Vasiliou, D. Mastropaolo, J. A. Potenze, and H. J. Schugar, "Molecular Structure and Magnetic Properties and μ-Dihydroxo-bis [2,6-pyridinedicarboxylatoaquoiron (III)] and μ-Dihydroxo-bis [4-hydroxo- 2,6-pyridinedicaroboxylatoaquoiron (III)] Tetrahydrate", **Journal of the American Chemical Society *98***, (1976) 1425.

4. C. C. Ou, D. A. Powers, J. A. Thick, T. R. Felthouse, D. N. Henrickson, J. A. Potenze, and J. H. Schugar, "Molecular Structure and Magnetic Properties of Trans-Bis (L-methioninato) copper (II), $Cu(C_5H_{10}NO_2S)_2$", **Inorganic Chemistry *17***, (1978) 34.

5. D. Mastropaolo, D. A. Powers, J. A. Potenze, and H. J. Schugar, "Crystal Structure and Magnetic Properties of Copper Citrate Dihydrate, $Cu_2C_6H_4O_7.2H_2O$", **Inorganic Chemistry *15***, (1976) 1444.

6. D. A. Powers, "Chemical and Physical Processes of Reactor Core Meltdown", Chapter 4 in **Core-Meltdown Experimental Review**. W. B. Murfin, Ed., SAND74-0382, Sandia Laboratories, Albuquerque, NM, March 1977.

7. D. A. Powers, "Empirical Models for the Thermal Decomposition of Concrete", **Transactions of the American Nuclear Society *26***, (1977) 401.

8. D. A. Powers, "Large-Scale Melt/Concrete Interactions Tests", **Transactions of the American Nuclear Society *26***, 400 (1977).

9. J. F. Muir, D. A. Powers, and D. A. Dahlgren, "Studies on Molten Fuel Concrete Interactions", **Proceedings of the International Conference on Fast Reactor and Related Physics** (Chicago, October 1976) **CONF**-761001, Volume IV, p. 2095, August 1977.

10. D. A. Dahlgren, D. A. Powers, J. F. Muir, and B. M. Butcher, "Experimental Results of the Interaction of Molten Core Materials with Concrete", **Proceedings of the Specialists Meetings on the Behavior of Water Reactor Fuel Elements Under Accident Conditions** (Spating, Norway, September 1976) CSNI Report No. 13, March 1977.

11. D. A. Dahlgren, L. D. Buxton, J. F. Muir, W. B. Murfin, L. S. Nelson, and D. A. Powers, "Molten LWR Core Material Interactions with Water and with Concrete", **Proceedings of**

the Topical Meeting on Thermal Reactor Safety (Sun Valley, ID, July-August 1977).

12. D. A. Powers, D. A. Dahlgren, J. F. Muir, and W. B. Murfin, **Exploratory Study of Molten Core Materials/Concrete Interactions July 1975 - March 1977**, SAND77-2042, Sandia Laboratories, Albuquerque, NM February 1978.

13. D. A. Powers, "Interactions between Molten Nuclear Reactor Core Materials and Structural Concrete", **Revue Internationale des Hautes Temperatures et des Refractaires 16** (1979) 73.

14. D. A. Powers, **Sustained Molten Steel/Concrete Interactions Tests--Preliminary Report on the Feasibility of Experimental Techniques**, SAND77-1423, Sandia Laboratories, Albuquerque, NM, June 1978.

15. D. A. Powers, "Sustained Molten Steel/Concrete Interactions Tests", **Proceedings of the Post-Accident Heat Removal Information Exchange**, November 2-4, 1977, Argonne National Laboratories, p. 433, ANL-78-10.

16. D. A. Powers, "Influence of Gas Generation on Melt/Concrete Interactions", **Thermodynamics of Nuclear Materials 1979**, Vol. II, Paper IAEA-SM-236/48 p. 351, International Atomic Energy Agency, Vienna, 1980.

17. A. S. Benjamin, D. J. McCloskey, D. A. Powers, and S. A. Dupree**, Spent Fuel Heatup Following Loss of Water During Storage**, SAND77-1371, Sandia Laboratories, Albuquerque, NM, March 1979.

18. D. A. Powers, "A Survey of Melt Interactions with Core Retention Materials", **Proceedings of the International Meeting on Fast Reactor Safety Technology**, Seattle, WA, August 1979), Volume I, p. 379, American Nuclear Society, LaGrange Park, IL 1979.

19. T. Y. Chu, A. G. Beattie, W. D. Drotning, and D. A. Powers, "Medium Scale Melt-Sodium Fragmentation Experiments", **Proceedings of the International Meeting on Fast Reactor Safety Technology** (Seattle, WA, 1979), Vol. II, p. 742, American Nuclear Society, LaGrange Park, IL 1979.

20. M. M. Karnowsky, R. M. Biefeld, R. P. Clark, and D. A. Powers, "The Li_2CrO_4 Binary Phase Diagram", **Thermochimica Acta *40***, (1980) 398.

21. M. P. Sherman, M. Berman, J. C. Cummings, G. W. Perkins, D. A. Powers, P. O. Bieniarz, and O. R. Green, **The Behavior of Hydrogen During Accidents in Light Water Reactors**, NUREG/CR-1561, SAND80-1492, Sandia National Laboratories, Albuquerque, NM, August 1980.

22. D. A. Powers, "Hydrogen Effervescence and the Pressurizer Level Detector", in

Appendix II.10 of **Three Mile Island - A Report of the Commissioners and to the Public**, M. Rogovin, Director, Volume II, part 2, p.803.

23. D. A. Powers, "Status of the Reactor Core Based on Fission Product Analysis", in Appendix II.10 of **Three Mile Island - A Report of the Commissioners and to the Public**, M. Rogovin, Director, Volume II, part 2, p.803.

24. D. A. Powers, "Plausible Conditions of the TMI-2 Core" (invited) **Transactions American Nuclear Society *34*** (1980) 563.

25. D. A. Powers, "A Review of Steam Oxidation of Steels - the Forgotten Source of Hydrogen", **Proceedings of the Workshop on the Impact of Hydrogen on Water Reactor Safety,** NUREG/CR-2017, SAND81-0661, Sandia National Laboratories, Albuquerque, NM.

26. W. B. Murfin and D. A. Powers, "Interaction of the Melt with Concrete and MgO", chapters in **Report of the Zion/Indian Point Study**: Volume I, NUREG/CR-1410, SAND80-0617/1, Sandia National Laboratories, Albuquerque, NM, August 1980.

27. J. A. Thich, B. H. Toby, D. A. Powers, J. A. Potenze, and H. J. Schugar, "Magnetic Properties of $K_5(H_2O)_3(SO_4)_6Fe_3O.6H_2O$, A Sulfate Analog of the Trimeric Basic Iron (III) Carboxylates", **Inorganic Chemistry *20***, (1981) 3314.

28. D. A. Powers and F. E. Arellano, **Large-Scale, Transient Test of the Interaction of Molten Steel with Concrete**, NUREG/CR-2282, SAND81-1853, Sandia National Laboratories, Albuquerque, NM, January 1982.

29. D. A. Powers and F. E. Arellano, **Direct Observation of Melt Behavior During High Temperature Melt/Concrete Interactions**, NUREG/CR-2283, SAND81-1754, Sandia National Laboratories, Albuquerque, NM, January 1982.

30. R. K. Hilliard, R. P. Johnson, and D. A. Powers, UNITED States Position Paper on Sodium Fires, Design and Testing", **Summary Report, Specialists Meeting on Sodium Fires, Design and Testing**, International Working Group on Fast Reactors, International Atomic Energy Agency, IWGFR/43, 1982.

31. D. A. Powers and F. E. Arellano, **Erosion of Steel Structures by High Temperature Melts**, NUREG/CR-2284, SAND81-1755, Sandia National Laboratories, Albuquerque, NM, June 1983.

32. D. A. Powers and F. E. Arellano**, High Temperature Melt Attack on Steel and Urania-Coated Steel**, NUREG/CR-3366, SAND83-1350, Sandia National Laboratories, Albuquerque, NM, April 1984.

33. D. A. Powers, "Erosion of Steel Structures by High Temperature Melts", **Proceedings of the ANS 1983 Winter Meeting on Nuclear Thermal Hydraulics, Transactions**

American Nuclear Society *45* (1983), 189.

34. D. A. Powers, J. E. Brockmann, D. R. Bradley, and W. W. Tarbell, "The Role of Ex-Vessel Interactions in Determining the Severe Reactor Accident Source Term for Fission Product", paper 11.8 **Proceedings ANS/ENS Topical Meeting on Severe Reactor Accident Evaluation**, Cambridge, MA August 28 - September 1, 1983.

35. A. R. Taig, C. D. Leigh, D. A. Powers, J. L. Spring, J. C. Cunnane, H. I. Avci, P. Baybutt, and J. A. Gieseke, "Fission Product Behavior Modeling in Risk Analyses--An Assessment of the Relevant Phenomena", **Proceedings International Meeting LWR Severe Accident Evaluation**, Volume 1 (1983) pp.2.5/1 to 2.5/10.

36. D. A. Powers, "Erosion of Steel Structures by High Temperature Melts", **Nuclear Science and Engineering 88**, (1984) 357.

37. D. A. Powers, **Behavior of Control rods During Core Degradation: Pressurization of Silver-Indium-Cadmium Control Rods**, NUREG/CR-4401, SAND85-0459, Sandia National Laboratories, Albuquerque, NM, September 1985.

38. D. A. Powers and J. E. Brockmann, "A Mechanistic of Release of Radionuclides and Generation of Aerosols During Reactor Core Melt Interactions with Concrete", **Proceedings of the 16th Annual Meeting of the Fine Particle Society**, Miami Beach, FL, April 1985.

39. R. J. Lipinski, R. K. Mast, D. A. Powers, and J. V. Walker, **Uncertainty in Radionuclide Release Under Specific LWR Accident Conditions Volume 1 Executive Summary**, SAND84-0410, Col. 1, Sandia National Laboratories, Albuquerque, NM, May 1985.

40. D. A. Powers, "VANESA Sensitivity Study" appendix L, **Uncertainty in Radionuclide Release Under Specific LWR Accident Conditions Volume 2 TMLB Analyses**, SAND84-0410 Vol. 2, Sandia National Laboratories, Albuquerque, NM, February 1985.

41. D. A. Powers, J. E. Brockmann, and A. W. Shiver, **VANESA: A Mechanistic Model of Radionuclide Release and Aerosol Generation During Core Debris Interactions with Concrete**, NUREG/CR-4308, SAND85-1370, Sandia National Laboratories, Albuquerque, NM, July 1986.

42. D. A. Powers, with others, **Uncertainty in Radionuclide Release Under Specific LWR Accident Conditions Volume 3 S2D Analyses**, SAND84-0410 Vol. 3, Sandia National Laboratories, Albuquerque, NM, April 1985.

43. D. A. Powers, "Sensitivity of the VANESA Model", Appendix D in **Uncertainty in Radionuclide Release Under Specific LWR Accident Conditions Volume 4 TC Analyses**, SAND84-0410 Vol. 4, Sandia National Laboratories, Albuquerque, NM,

December 1985.

44. D. A. Powers, Isotopes, Elements and Chemical Classes", Chapter 2, "Release of Fission Products and Generation of Aerosols During In-Vessel Stages of a Severe Accident", Chapter 3, and "Fission Product Release and Aerosol Generation Within the Reactor Containment", Chapter 4 in **Fission Product Behavior During Severe LWR Accidents - Modeling Recommendations for the MELCOR Code System**, Sandia National Laboratories, Albuquerque, NM NUREG/CR-4481, SAND84-2743.

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APPENDIX B: DETAILED PIRT TABLES

This appendix presents the detailed tables of the Phenomena Identification and Ranking Table (PIRT) exercise.

Table B-1: Summary of PIRT Results (1 of 7)

Phenomenon	Importance Rankings			State of Knowledge Rankings						
	Scenario 1: Pool Fire	Scenario 2: Spray Fire	Comments	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data	Comments
1. Pool Fire Surface Burning										
A. Radiation Flux from Pool Burning Surface	L	L		X	X	X	X	X	X	
B. Radiation Flux to Pool Burning Surface	L	L	This is less important than the phenomenon radiation flux from the surface.	X	X	X	X	X	X	
C. Mass Burning Rate	H3	L	The mass burning rate is highly important for the pool fire and low importance for the spray fire.	M	L	M	H	M	M	The models for this phenomenon are decent if all the input are available. The complicated issues are the surface reaction with the oxide deposition.
D. Pool Heating Rate	H2	L	The high importance ranking for the pool fire is specific to the initial heat up from feedback.	M	L	M	H	M	M	
E. Mass Burning Rate if Radiation is Important	H1	L	The high importance for the pool fire is based on that this phenomenon affects the heat release rate. The low importance ranking for the spray fire is presuming that the sodium spray is not depositing on the ground.	L	L	L	L	L	L	The uncertainties with this phenomenon are the sodium optical properties. The absorption is largely reflective.
F. Conduction/Convective Flux	H2	L		H	H	H	NA	L	L	
G. Near Surface Size and Distribution of Aerosol Particles	H2-M	NA	This phenomenon was ranked by the panel with a state of knowledge range from medium to H2 due to the uncertainty associated with the near field distribution.	L	L	L	L	L	L	There is far field data from pervious experimental work that gives information about the far field distribution. The lack of information is for the near field data.
H. Damaged State (Complex Surfaces)	H3-H1	L	It was noted that the rankings could be different depending where the sodium pool or spray is located (concave or convex surface).	X	X	X	X	X	X	
I. Gaseous Products of Metal Reaction and Velocity of Gaseous Products Coming off of the Surface	L	L	Note that the hydrogen production was handled in a separate phenomenon under sodium-concrete interactions.	X	X	X	X	X	X	
J. Source of Sodium Aerosols	H3	NA		L	L	L	L	L	L	
K. Treatment of the Oxide Crust	L	L	Some of the questions that were noted for this phenomenon were: (1) if the crust on the pool surface affects the oxygen transport does this affect the quenching and (2) will the sodium ignition temperature be higher with the oxide crust?	X	X	X	X	X	X	

Table B-2: Summary of PIRT Results (2 of 7)

Phenomenon	Importance Rankings			State of Knowledge Rankings						
	Scenario 1: Pool Fire	Scenario 2: Spray Fire	Comments	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data	Comments
L. Film Thickness in Sodium Pool Spreading (Viscosity Issue)	H3 to M	H	It was noted that there was a lot of research done by George Greene in this area. The range in importance ranking for scenario 1 for this phenomenon emphasizes the uncertainty associated with it.	M	L	L	M	L	L	The capillary spread models was used with some of the recent Japanese discovery experiments which did not work so well.
M. Burning on Surface	L	H		L	L	M	M	L	L	
N. Pressure Effect on Combustion (Vapor)	L	L		X	X	X	X	X	X	
2. Plume Dynamics										
A. Momentum Transport (i.e. Velocity Field)	H	H	This phenomenon was ranked as high importance because sodium will not burn without oxygen. How oxygen is transported to the source is important.	H	H	H	NA	H	NA	These models are in the literature.
B. Turbulence Production	M	M		H	H	M	M	H	NA	
C. Mixing (Turbulence Model), Oxidizer Transport	H	H	The high importance is based on that this phenomenon determines the combustion rate.	H	H	H	NA	H	NA	
D. Temperature Distribution (Fluctuations)	M	M	It was noted that this phenomenon was specific to the heat balance of the room and if that had significant contributions.	H	H	M	M	H	NA	
3. Spray Dynamics										
A. Prediction of Droplet Particle Average Velocity	L	H	The high importance for Scenario 2 is specific to the difference in the spray fire versus a pool fire. It is important to predict the initial velocity to know when the droplets will hit a surface. Predicting the variation of velocity is not as important.	H	H	H	NA	H	NA	
B. Prediction of Droplet Particle Velocity Distribution/Range	L	L		X	X	X	X	X	X	
C. Prediction of Single Droplet Particle Average Size	L	H		M	M	L	L	L	L	Some of the physics that are not well understood are the fraction of oxide that goes off the droplet and how much comes back and what the source of variation is.

Table B-3: Summary of PIRT Results (3 of 7)

Phenomenon	Importance Rankings			State of Knowledge Rankings						
	Scenario 1: Pool Fire	Scenario 2: Spray Fire	Comments	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data	Comments
D. Prediction of Droplet Particle Size Distribution/Range	L	M		M	M	L	L	L	L	
E. Droplet Particle Velocity Variation/Range	L	M	The panel noted that the range will varry according to droplet size.	M	M	L	L	L	L	
F. Particle Clouds over Multiple Control Volumes (Basic Capability)	L	L		X	X	X	X	X	X	
G. Particle Clouds over Multiple Control Volumes (Effects of Solid Interactions/Flow Strain)	L	L		X	X	X	X	X	X	
H. Basic Evaporation/Combustion Models	L	H		H	H	M	NA	H	NA	
I. Finite-Slip Corrections to Evaporation/Combustion Models	L	M	There might not be a lot of droplet deformation if surface tension is high.	H	H	H	H	H	H	
J. Transition to Group Combustion Mode	L	L		X	X	X	X	X	X	
K. Multi-Component Droplet Capabilities	L	L		X	X	X	X	X	X	
L. Source for Sodium Aerosols	L	H	This phenomenon is related to the multi-component interactions. What is the fraction of small particles that come off the falling sodium.	L	L	L	L	L	L	
M. Chemical Kinetics of Sodium Combustion	L	L		X	X	X	X	X	X	
N. Molecular Diffusion Coefficient Across Diffusion Flame	L	H	This phenomenon is of high importance because it drives the burning rate for droplets.	H	H	H	NA	M	L	These state of knowledge rankings have a high uncertainty associated with them.
O. Gas-Band Radiation from Diffusion Flames	L	L	This was ranked low because the panel does not expect gas species to complicate transport.	X	X	X	X	X	X	
P. Radiation from Aerosols in Diffusion Flame	L	M		L	L	L	L	L	L	Effective emission of burning aerosol cloud around the droplet is one of the parameters that is complicated to model.
Q. Mass Flux of Aerosols through Diffusion Flame (i.e. diff-diff)	L	M	This phenomenon is a subcomponent of the radiation from aerosols in a diffusion flame. Specifically aerosols going through diffusion flames and how long the aerosols would be at high temperatures.	L	L	L	L	L	L	
R. Sodium Particle Collision	L	L		X	X	X	X	X	X	
S. Inertial Impact of Molten Sodium	L	M	This phenomenon was in context of atomization.	M	L	M	L	M	L	

Table B-4: Summary of PIRT Results (4 of 7)

Phenomenon	Importance Rankings: Scenario 1: Pool Fire	Importance Rankings: Scenario 2: Spray Fire	Importance Rankings: Comments	State of Knowledge Rankings: Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data	State of Knowledge Rankings: Comments
T. Burning on Surface	L	H		L	L	M	M	L	L	
4. Aerosol Dynamics										
A. Source of Sodium Aerosols	H	NA		L	L	L	L	L	L	
B. Thermopheric Transport of Aerosols	H	H	It was noted that obtaining the thermal gradient is important.	M	M	L	M	L	M	Eastimating the uncertainty in agglomerate particles for modeling and theory for spheres and agglomertates contaiing high void space and relevant paramter detemination could be difficult. An empirical approach may be best for testing to determine how prototypically generated sodium fire aerosols transport in thermal gradients.
C. Radiation to/from Individual Aerosols	M	M		X	X	X	X	X	X	
D. Electrical Properties	H	H	Obtaining the charge on particles and the electric fields in the facility are important. This is possible as long as the charge doesn't produce a space charge sufficient to cause cloud expansion or there will be no electric fields. Image force is what will enhance deposition and this only acts over a few tenths of particle diameters from the surface.	M	M	L	M	L	M	The importance here is determining if the aerosol is charged and what measurements are needed to determine this charge level.
E. Turbulent Inertial Deposition	M	M		X	X	X	X	X	X	
F. Gravitational Settling	H	H	This phenomenon was ranked as high importance due to the figure of merit pertaining to electrical equipment vulnerability. Big particles move down quickly but smaller particles move around and can settle on equipment and possibly block filters and ventilation.	H	H	M	H	M	H	We need to know the particle shape factor to determine the settling. There is data available on the fractal dimension of particles generated in this manner.
G. Interception	M	M		X	X	X	X	X	X	
H. Electro-Static Deposition	M	M		X	X	X	X	X	X	

Table B-5: Summary of PIRT Results (5 of 7)

Phenomenon	Importance Rankings			State of Knowledge Rankings						
	Scenario 1: Pool Fire	Scenario 2: Spray Fire	Comments	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data	Comments
I. Aerosol Agglomeration	H	H	Agglomeration determines the particle size and will as such influence depositon and transport behavior.	H	H	M	M	M	M	There are coagulation kernals for agglomeration of fractal particles and data from the silica and carbon black industries that should have some applicability.
J. Hydrolysis of Peroxides	M	M		X	X	X	X	X	X	
K. Aerosol Particle Charging	U	U	The panel is uncertain on the importance of this phenomenon in regards to the figure of merit. Particle charging could form conduction pathways across electronics and change electrical permittivity of air.	X	X	X	X	X	X	
L. Sodium Carbonate Deposition	H	H	Aerosol deposition will not likely be differentiated by speciation as it is likely that the particles will contain multiple species depending on their age and history.	M	M	M	M	M	M	For generic deposition, the state of knowledge varies by mechanism as for speciation dependence, there is very little information for our application.
M. Sodium Hydroxide Aerosol Deposition	H	H		M	M	M	M	M	M	For generic deposition, the state of knowledge varies by mechanism as for speciation dependence, there is very little information for our application.
N. Sodium Peroxide Aerosol Deposition	H	H		M	M	M	M	M	M	For generic deposition, the state of knowledge varies by mechanism as for speciation dependence, there is very little information for our application .
O. Thermal Interaction of Deposit Layer for Aerosol Mixture (*i.e.* an Effective Conductivity Model or other Treatment)	L	L		X	X	X	X	X	X	
P. Effective Emissivity of Deposit Layer	L	L		X	X	X	X	X	X	
Q. Thermophoresis Effect on Deposition Flux	H	H		M	M	L	M	L	M	
5. Radiation Heat Transfer										
A. Radiation to/from Individual Aerosols	M	M		X	X	X	X	X	X	

Table B-6: Summary of PIRT Results (6 of 7)

Phenomenon	Importance Rankings			State of Knowledge Rankings						
	Scenario 1: Pool Fire	Scenario 2: Spray Fire	Comments	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data	Comments
B. Radiation Transport for Absorption/Emission	H	H	For Scenario 1 (pool fire) the importance for this phenomenon will depend on what the sodium is sitting on. If the substrate is catastrophically damage then the pool will fall to another surface, possibly concrete. The thermal load from gas phase and/or pool fire could contribute to take failure of equipment. For Scenario 2, the phenomenon was ranked high because if the sodium spray fell on a surface early in the accident, this phenomenon would play an important role in evuluating the fire scenario.	H	H	M	M	H	NA	The complication with predicting this phenomenon is the uncertainty associated with the composition of the sodium oxide layer.
C. Radiation Transport for Scattering	H	H		H	H	L	M	H	NA	Importance ranking for Scenario 1
				H	M	L	M	H	NA	Importance ranking for Scenario 2.The code adequacy would be high if you can use MIE scattering with well know spheres.
D. Lagrangian Absorption/Emissive Coupling with Radiation Field	L	H		H	L	NA	NA	NA	NA	
E. Spectral Dependence of Radiation Field	U	U		H	L	L	M	H	NA	The code adequacy was mentioned to be very low.
F. Lagrangian Scattering Coupling with Radiation Field	L	H		H	L	L	M	H	NA	
G. Overall Joint-Temperature-Absorption Coefficient Distribution	M	M	The panel noted that the medium ranking has a high uncertainty specifically to the hydrodynamic coupling of cloud effects.	M	L	L	L	L	L	
H. Gas-Band Radiation from Diffusion Flames	L	L	The panel does not expect gas species to complicate transport.	X	X	X	X	X	X	
6. Concrete-Sodium Interactions										
A. Hydrogen Production	H	H		M	L	L	M	L	L	
7. Liquid Molten Jet										
A. Liquid Splashing on Solid	H	H	This is important based on the presumption that it is likely that some unburned sodium will reach the floor. This phenomenon is specific to the liquid sodium coming in contact with a hard surface.	M	L	M	M	M	M	

Table B-7: Summary of PIRT Results (7 of 7)

Phenomenon	Importance Rankings			State of Knowledge Rankings						
	Scenario 1: Pool Fire	Scenario 2: Spray Fire	Comments	Model Adequacy	Code Adequacy	Available Input Data	Feasibility of Getting New Input Data	Available Validation Data	Feasibility of Getting New Validation Data	Comments
B. Liquid into Pool	H	H	This phenomenon is specific to the liquid sodium going into another liquid. For this case, liquid sodium going into a pool of liquid sodium.	L	L	L	H	L	M	The uncertainties are with the rate of spreading of the sodium pool and the physics of quenching the sodium pool in regards to heat transfer balance.
C. Liquid Jets, Jet Breakup	L	H		M	M	H	NA	H	NA	
D. Vapor Jet into Liquid	L	L		X	X	X	X	X	X	
E. Spray Formation in Vapor Jet	L	L		X	X	X	X	X	X	
8. Chemistry (Needed for Quenching)										
A. Burning on Surface	L	H	This phenomenon was specific to the sodium hitting an object and burning. The low ranking for the pool fire scenario is on the presumption that a sodium pool has formed on the ground.	L	L	M	M	L	L	
B. Condensed-Phase Reactions with Substrate	H	H	The high importance ranking for this phenomenon are based on the potential for a sodium-concrete reaction which will produce hydrogen gas. The high importance is also based on the potential reaction of a spray fire with the cable insulation.	M	L	L	L	L	L	
C. Wetting/Sticking Properties of Sodium on Expected Surfaces	H	H	This phenomenon was specific to the particle boundary interaction; how much of the sodium will stick to a surface versus falling to the ground.	M	L	U	U	U	U	The uncertainty rankings are based on the unknown surface energies of the touching surfaces.

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